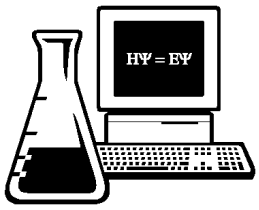
AMPAC

Graphical User Interface

User's Manual



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Printed in the USA *Revised: 8/11/97* *Version 6.0*

Contents

Welcome to the *AMPAC GUI*

The ***AMPAC GUI*** is an advanced graphical user interface designed to be used with AMPAC and GAUSSIAN-94 to make calculations easier, quicker and more efficient. The ***AMPAC GUI*** features easy AMPAC and GAUSSIAN-94 calculation set up and three dimensional molecular visualization.

Structure of the Manual

This *User's Manual* is designed to be used either as a hands-on tutorial or as a reference. The information in this guide starts with the basics of the ***AMPAC GUI***, which begins with running it for the first time, continues with descriptions of its components, and then includes examples detailing how various calculations are set-up, executed, and the results visualized.

Hint>

It is not necessary to read this guide sequentially The user can skip directly to the information needed. To help enhance computations or save steps in carrying out your tasks, quick tips and hints are identified by the icon at the left.

Audience for the Manual

This *User Manual* is designed to familiarize beginners as well as advanced users of AMPAC with the use, features, and components of the ***AMPAC GUI***.

Even if you are new to AMPAC or GAUSSIAN-94, setting up and running jobs through the ***AMPAC GUI*** will be easy because the windows and dialog boxes in the GUI will guide you through the occasionally complex procedures, setting a number of common options as defaults along the way.

For advanced users of AMPAC and GAUSSIAN-94, the ***AMPAC GUI*** presents a more rapid graphical approach to doing calculations within the context of familiar procedures.

Contents of Manual

This *User's Manual* is designed to follow how users will normally interact with the ***AMPAC GUI***. Chapters synopses follow.

Chapter 1, Getting to Know the ***AMPAC GUI*** Presents a summary of features, describes the basic components of the ***AMPAC GUI***, provides step-by-step start-up instructions, and contains quick reference tables of [BUILDER]and [WORK AREA] options.

Chapter 2, Building Molecules Contains descriptions of the [BUILDER]and [WORK AREA] options, and provides molecule building examples demonstrating the function of the ***AMPAC GUI.***

Chapter 3, Setting Up and Running AMPAC and GAUSSIAN-94 Computational Jobs Describes procedures for creating, running, and viewing AMPAC files via options available through the ***AMPAC GUI*** •CALCULATE• menu items and CURRENT JOBS manager.

Chapter 4, Visualizing Results Describes the •RESULTS• menu and its options which enable you to examine the results of your AMPAC and/or GAUSSIAN-94 calculations.

This manual contains many example screen shots from the ***AMPAC GUI*** product. Be aware that their appearance may vary slightly according to the window manager program (e.g. Motif, twm, and so on) you are using and other specific configuration settings of your computer system. Note also that the ***AMPAC GUI*** will appear in color on your screen, not black and white.

1 Getting to Know the *AMPAC GUI*

This chapter provides an overview of the ***AMPAC GUI***'s features and capabilities. The ***AMPAC GUI*** is a graphical user interface(GUI) designed to help you prepare input for submission to AMPAC and GAUSSIAN-94 and to examine graphically the output produced from such calculations. The ***AMPAC GUI*** is not integrated with the computational modules of AMPAC and/or GAUSSIAN-94, but is a front-end/back-end processor to aid in the use of these programs.

For systems that support OpenGL, the ***AMPAC GUI*** runs using the OpenGL graphics language for enhanced visual quality and speed. For other systems, the ***AMPAC GUI*** is programmed to comply with the Motif/X-Windows (X11.R4) graphical environment and runs under most modern operating systems.

What the *AMPAC GUI* Can Do

The ***AMPAC GUI*** is a powerful tool that allows you to easily build molecules, efficiently set up many types of calculations, and view many types of AMPAC and GAUSSIAN-94 results graphically. Results that can be viewed include the following:

- Optimized molecular structures and geometric parameters
- Unpaired charge densities
- Molecular orbitals
- Electron density surfaces from any computed density
- Electrostatic potential surfaces
- Animation of the normal modes corresponding to vibrational frequencies

Through its advanced visualization capabilities, the ***AMPAC GUI*** allows you to rapidly construct even very large molecules, then rotate, translate and zoom in on these molecules through simple mouse operations.

The ***AMPAC GUI***'s two main windows, the [BUILDER]and [WORK AREA], have pull-down menus that facilitate your choices from the available options. The structure of these windows and their pull-down menus make the ***AMPAC GUI*** easy to learn and use.

Introducing the Basics

Following is an overview of the basic components of the ***AMPAC GUI***. Detailed descriptions are provided in the chapters that follow. Examples are provided in the section on *Building Molecules* in Chapter 2.

Windows and Options

You will be using the ***AMPAC GUI***'s [BUILDER] and [WORK AREA] windows to construct and manipulate molecules of interest. The [BUILDER] window contains options for constructing and manipulating molecules in the [WORK AREA].

The main [WORK AREA] palette contains pull-down menus that provide options for controlling the ***AMPAC GUI***'s interaction with input and output files. You can set program options by clicking on the appropriate pull-down menu items.

Dialog boxes are presented when the ***AMPAC GUI*** needs to read a file, save a file, or set program options. The [OPEN] and [SAVE] dialog boxes help you navigate file structures to locate files and directories. Select an item by double-clicking on its name or single-clicking and hitting the OK button.

Working with a Three-button Mouse

Interaction with molecules is designed around the movements of a three-button mouse. The functions of the mouse buttons are described in the following table:

Mouse Button	Action	Function
Left	Click	Selects or inserts item.
	Drag Left/Right	Rotates about Y axis.
	Drag Up/Down	Rotates about X axis.
Center	Drag	Translation of molecule on screen.
Right	Drag Left/Right	Rotates about Z axis.
	Drag Up /Down	Zooms and recedes size.

Three-button mouse functions

Holding down the tab key limits mouse action to the distinct (unbonded) fragment nearest the pointer.

The AMPAC GUI Quick Start

This section provides a quick guide for starting the ***AMPAC GUI*** and a general overview of how to use the ***AMPAC GUI***. For more detailed information and descriptions, refer to subsequent chapters. On-line, context-sensitive help is also available in virtually every window and dialog box.

Launching *THE AMPAC GUI*

You've installed the ***AMPAC GUI*** according to the provided instructions. Now how do you activate it? The steps listed below (for various versions of the *Unix* operating system) are designed to get you started. Once in the ***AMPAC GUI***, you will find that capabilities and options are available to you with just a click of the mouse button.

1. If you're displaying the ***AMPAC GUI*** on the same machine that the ***AMPAC GUI*** is executing on, type the following to start the application:

```
% agui
```

If the ***AMPAC GUI*** resides on a remote host, execute the following command on the local host:

```
% xhost remote-hostname
```

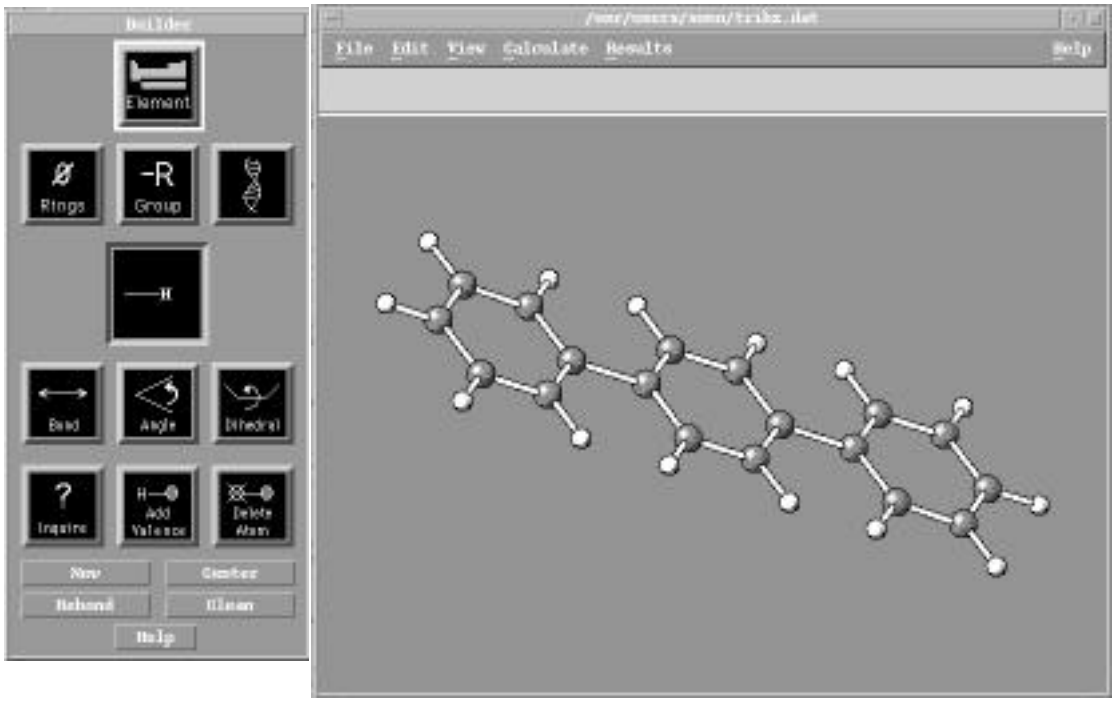
Log on to the remote host and type the following to display on the local host:

```
% setenv DISPLAY local-hostname:0.0
% agui
```

To force the ***AMPAC GUI*** to run in X mode on an OpenGL system, type the following:

```
% xagui
```

2. *Click on the copyright window to dismiss it.* The [BUILDER]and [WORK AREA] windows become easily accessible and ready for use.



3. *Reposition the windows on your screen.* Place the cursor on the task bar of either the [BUILDER] or [WORK AREA] window to move it. Hold down the mouse button while dragging the window to the new location, then release the button. You may want to resize the [WORK AREA] window.

You can easily go back and forth between the [WORK AREA] *and* [BUILDER]*windows not only while you're constructing new structures (either atom by atom or from fragments) but also while examining and manipulating previously-computed molecules.*

4.a *To create a new molecule:*

New molecules can be constructed either from fragments (AM1 preminimized structures) or atom-by-atom. Generally, working with preminimized building blocks and using the GUI's features to perturb them for your particular problem is the best approach, but there are situations where atom-by-atom is better. In either case, the starting point is selecting a fragment (from the ELEMENTS, RINGS, GROUPS, or BIO fragments) or an atom type (ELEMENTS) from options on the [BUILDER] form. So, select an item to work with from the [BUILDER]. Go back to the [WORK AREA] window, place the pointer where you want you selection to be inserted and click the leftmost mouse button.

You can control the number of times the item you selected will appear on the [WORK AREA] *window by the number of times you click on the* [WORK AREA] *window. You don't need to go back to the* [BUILDER]*window each time. In other words, the GUI is in "INSERT" mode unless another mode is explicitly selected on the* [BUILDER]*window.*

4.b *To work with an existing molecule:*

Select the OPEN... option on the •FILE• menu and a dialog box that enables you to open various types of files is presented. Choose a file type from the list at the top of the dialog box, and only files of this type will be presented in the right scrolling information box. (The left box presents a list of directories that can be navigated to locate particular files.) Find the file you are interested in opening and either click on it twice or click on it once and click the OK button.

5. *Set up your **AMPAC** or GAUSSIAN-94 calculation.* Go to the •CALCULATE• menu on the [WORK AREA] window and select either AMPAC or G94 from the list of options. Select various options as you like, and submit the file from the dialog box using the SUBMIT button on those forms.

6. When the job has completed, examine the results of your calculation through options available in the •RESULTS• menu.

The AMPAC GUI Quick Reference

Following are reference tables summarizing the ***AMPAC GUI*** options and functions. Refer to later chapters for detailed descriptions of these options.

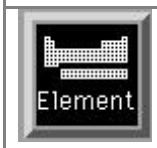
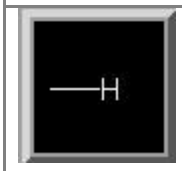
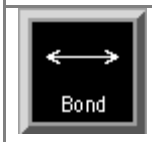
Quick Reference Table of [WORK AREA] Window Options

MENU	OPTION	DESCRIPTION
FILE	Provides the following options for creating, modifying, and saving structures:	
	New	Provides an empty screen for starting a new file. Clears the screen and resets all options to default. (You will be prompted to save any existing structure.)
	Open	Allows you to open files supported by the ***AMPAC GUI***. Has a dialog box that allows you to set the file filter type and append a structure to the molecule on the screen. (You will be prompted to save any existing structure.)
	Save	Allows you to save the molecule on the screen to a file with a format selected in the [SAVE] dialog box.
	Append	Adds a previously-saved structure to the structure in the [WORK AREA] window.
	Save Prefs	Saves the settings on all dialog boxes to various preference files. These settings will be set as defaults and used on all subsequent launches of the ***AMPAC GUI***. Make sure that all the settings are the way you want them before selecting this option. *Caution: This is a permanent change.*
	Print	Produces a PostScript file containing a line-art image of the structure in the [WORK AREA] window. You can send this file to a PostScript-capable printer or export it to graphical editing software for inclusion in documents.
	Exit	Closes all the ***AMPAC GUI*** windows and terminates the application.

EDIT	Provides the following options for performing large, global editing tasks:	
	Undo	Reverses the previous editing action and maintains a list of 10 previous actions so you can trace complex editing schemes.
	Redo	Reverses the Undo selection. Maintains a list of previous 10 actions to allow you to trace complex editing schemes.
	Rebond	Recomputes the bound atoms, identifying bonded atoms based on a distance/nearest-neighbor algorithm.
	Clean	Adjusts molecular geometry according to a defined set of rules to more closely match chemical intuition.
VIEW	Provides the following options for managing and interacting with the display of molecules in the [WORK AREA] window, and for closing or opening the [BUILDER] window:	
	Add View	Opens additional [WORK AREA] windows, each with an independently adjustable view of the current molecule.
	Center	Adjusts molecular size to fit the screen and centers it in the [WORK AREA] window.
	Z-Matrix Editor	Allows you to change atom ordering, specify connectivity, and set optimization flags for later use in an AMPAC or GAUSSIAN-94 calculation.
	Hide/Show Builder	Closes or reopens the [BUILDER] window.
	Hide/Show Hydrogens	Toggles on and off the display of hydrogen atoms (if present) in the [WORK AREA] window.
	Hide/Show Dummy	Toggles on and off the display of dummy atoms (if present) in the [WORK AREA] window.
	Hide/Show Labels	Toggles on and off the display of atom numbers in the [WORK AREA] window according to the sequence number of the atom in the list of atoms. (Use with or without SYMBOLS.)
	Hide/Show Symbols	Toggles on and off the display of atomic symbols in the [WORK AREA]. (Use with or without LABELS.)
	Display Format	Allows you to select the display format of molecules in the [WORK AREA] window. The [MOLECULAR DISPLAY FORMAT] dialog box allows you to control the molecule's appearance in motion and while still.

CALCULATE	Provides the following dialog boxes used for setting options for GAUSSIAN-94 calculations and viewing current jobs:	
	AMPAC	Allows you to set options for creating an AMPAC input file and running an AMPAC job based on the molecular structure displayed in the [WORK AREA] window. The items in the pull-down menus are the default selections for the calculation.
	G94	Allows you to set options for creating a GAUSSIAN-94 input file and running a GAUSSIAN-94 job based on the molecular structure displayed in the [WORK AREA] window. The items in the pull-down menus are the default selections for the calculation.
	Current Jobs	Displays a list of currently running ***GUI***-initiated jobs.
RESULTS	Presents the following dialog boxes used for examining the results of calculations from various output files. Items not present in the file are disabled in the menu:	
	Summary	Provides the summary data of the results of the calculation after the .ARC (AMPAC), .OUT (AMPAC), or .LOG (GAUSSIAN-94) file is read in.
	Charges	Allows you to manage the display of partial charge density as computed by various AMPAC or GAUSSIAN-94 methods. Note that the atom colors selection displays the default atomic colors of the ***AMPAC GUI***.
	Vibrations	Displays calculated vibrational data available from the .OUT (AMPAC) , .LOG, .CHK, or .FCHK (GAUSSIAN-94) files as dynamic screen motions. A line spectra with vibrations and predicted intensities is also available.
	Surfaces	Displays surfaces that can be displayed by the ***AMPAC GUI***. These surfaces become available either after a .CUB (AMPAC or GAUSSIAN-94) file is opened, or after surfaces are produced via the Generate option.
	View File	Starts an editor session for a file read from disk.

Quick Reference Table of Builder Window Options

OPTIONS	DESCRIPTION
Element and Fragment Options	
	Allows insertion and replacement of various elements in the [WORK AREA] window. Click on an element, go to the [WORK AREA] window and click on an atom, and your selection will be added to the molecule. The Active Fragment window (described below) displays the selected item.
	Accesses a set of AM1 pre-minimized ring structures (the default is benzene). The Active Fragment window displays the selected item.
	Accesses a set of AM1 pre-minimized functional group fragments (the default is carbonyl). The Active Fragment window displays the selected item.
	Accesses a set of AM1 pre-minimized fragments used for biological research (the default is arginine). The Active Fragment window displays the selected item.
	This window is referred to as the Active Fragment window. It displays items selected through the ELEMENT, RINGS, GROUP, and BIO buttons. Its appearance changes depending on which option is selected. This is the largest box in the [BUILDER] window.
Modifying Structural Parameters	
	Opens the Bond SmartSlide™ when you click on the Bond button and highlight two atoms in the [WORK AREA] window. The interatomic distance is dynamically adjusted when you move the slider along the scale. Check one of the choices in the BOND SELECT area to change the bond type.
	Opens the Angle SmartSlide™ when you click on the Angle button and highlight three atoms. The initial value is set to the selected bond angle. The angle is dynamically adjusted when you move the slider along the scale.
	Opens the Dihedral SmartSlide™ when you click on the Dihedral button and highlight four atoms. When activated, the initial value is set to the dihedral angle. The dihedral angle is dynamically adjusted when you move the slider along the scale. The first atom selected manages the motion resulting from changing the slider value.
Note: You must press the OK button before any changes made on the SmartSlides™ are permanently applied to the structure.	

	Allows you to request geometric information directly from the [WORK AREA] window when you click on atoms. The resulting display depends on the number of atoms you select.
Valence Modification Functions	
	Attaches additional valences (shown as hydrogen atoms) to a selected center.
	Eliminates atoms and open valences (half bonds).
[BUILDER] Window Buttons	
New	Creates a new (empty) [WORK AREA] window and resets all dialog box options to default values. This option performs the same task as the item on the •VIEW• menu.
Center	Centers the image in the [WORK AREA] window and resizes the image to make the most efficient use of the workspace. This option performs the same task as the item on the •VIEW• menu.
Rebond	Identifies bonded atoms based on a distance/nearest-neighbor algorithm. This option performs the same task as the item on the •VIEW• menu.
Clean	Adjusts molecular geometry according to a defined set of rules to more closely match chemical intuition. This option performs the same task as the item on the •VIEW• menu.
Help	Provides on-screen information about [BUILDER] components.

2 Building Molecules

The [BUILDER]and [WORK AREA] windows are discussed in detail in this chapter. The last section of this chapter, *Molecule Building Examples*, provides examples that illustrate how the ***AMPAC GUI*** works.

See Chapter 3, *Setting Up and Running **AMPAC** and GAUSSIAN-94 Jobs* for a detailed description of the •CALCULATE• menu and its options, and Chapter 4, *Visualizing **AMPAC** and GAUSSIAN-94 Results*, for a detailed description of the •RESULTS• menu and its options.

Using the [Builder] Window

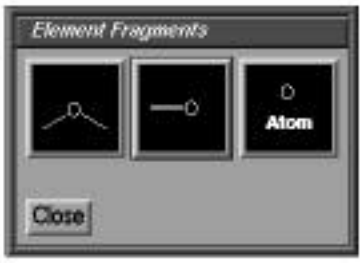
This section describes [BUILDER]window options (window shown at left). These options enable you not only to construct new structures either atom-by-atom or from fragments, but also to manipulate and examine previously-computed molecules.

Element and Fragment Options

[BUILDER]window options are controlled through the ELEMENT, RINGS, GROUP, and BIO buttons. These buttons tell the ***AMPAC GUI*** what to insert or replace when an atom is selected in the [WORK AREA] window. The ***AMPAC GUI*** begins and remains in the *insert/replace mode*, unless one of the options described below explicitly calls for it to act in a different manner.

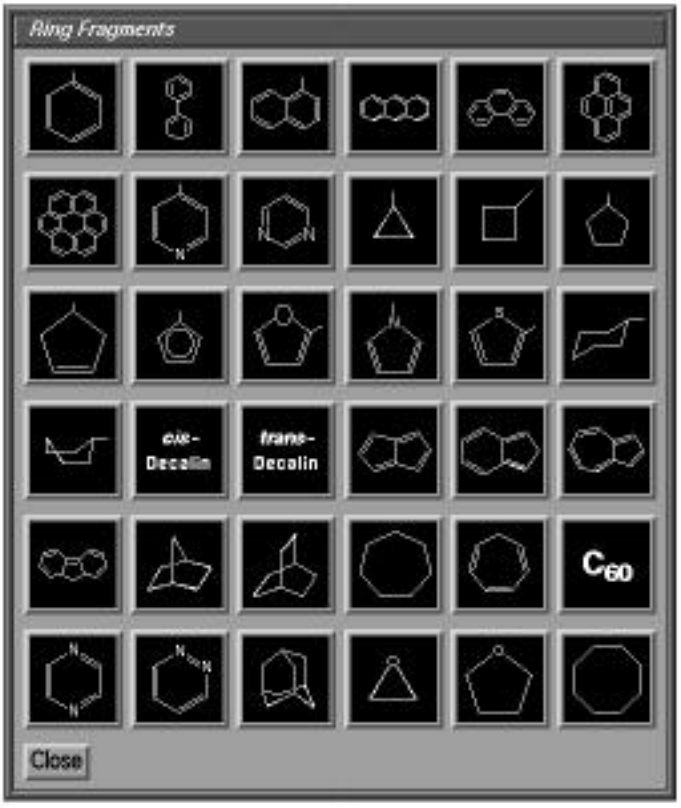
***Element*: Inserting/Replacing Elements**

This option allows the insertion/replacement of various elemental fragments. If you click on the ACTIVE FRAGMENT window after selecting an element, a set of possible coordination patterns for that element is presented, and the pattern that you select appears in the Active Fragment window.



At left is an example of the options available for oxygen (O).

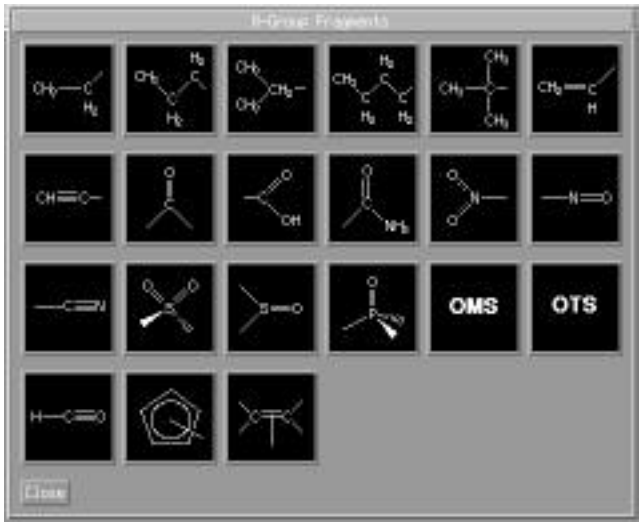
The last item is labeled "O atom". This fragment has special properties and activity. It may be placed *bare* (no valences) on the screen. A set of these could be used to sketch a molecule atom-by-atom. The REBOND option to connect atoms separated by appropriate distances. Another use for the bare atom fragment is for changing elemental identities. When a bare atom fragment is the active item, clicking on any atom in the current structure will change it to the selected element with no adjustment to valence.



***Rings*: Selecting Ring Structures**

Summons fragments for a set of AM1 pre-minimized ring structures. The default for RINGS is benzene. As with the ELEMENT button, if you click on the ACTIVE FRAGMENT window, the various stored structures (the form at left) are presented for selection. When one of them is chosen, it is placed in the ACTIVE FRAGMENT window.

The figure at the left shows the current set of predefined rings. The default ring is benzene.

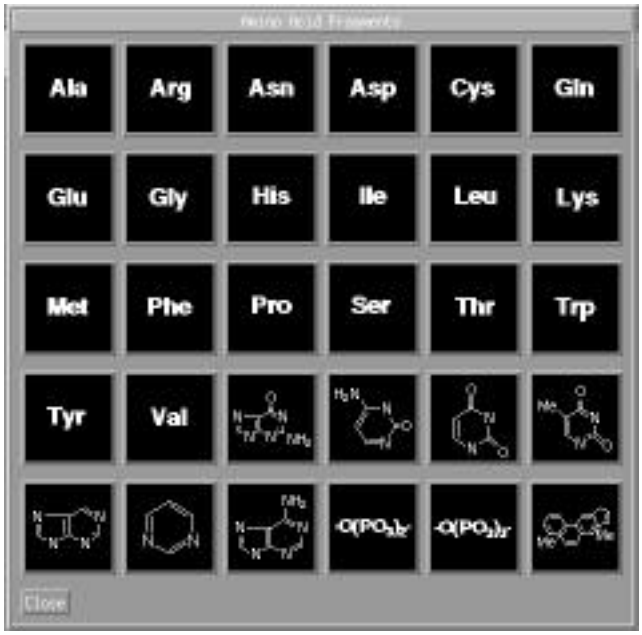


***Group*: Selecting Functional Group Fragments**

Displays a set of functional group fragments (AM1 pre-minimized structures). Again, as with ELEMENT or RINGS, if you click on the ACTIVE FRAGMENT window a set of structures is displayed on the window.

Note: Several of the fragments use non-traditional bonding arrangements. For example, one of these fragments includes a five-member ring with an open bond perpendicular to the plane of the ring. This is a cyclopentadienyl ligand for use in constructing organometallic (metallocene) systems.

The figure at the left shows the current set of predefined groups. The default group is carbonyl.



Bio: Selecting Fragments for Biological Applications

Summons a set of AM1 pre-minimized fragments useful to biological researchers (form at left). These fragments include the amino acids and various DNA bases.

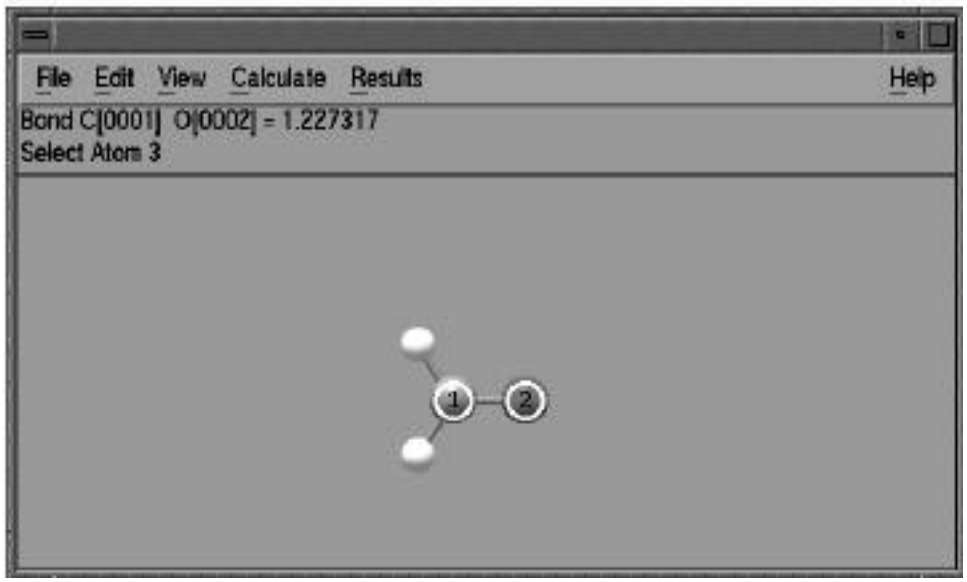
The figure at the left shows the current set of predefined biological fragments. The default group is the amino acid arginine.

Active Fragment Window: Display of Insertion/Replacement Items

The ACTIVE FRAGMENT window, located just below the RINGS, GROUPS, and BIO buttons, displays the currently selected item for insertion or replacement. Clicking on it brings up a palette of the available items of the currently-selected type.

Examining and Modifying Structural Parameters

The [BUILDER]window has the following options for examining and modifying the structural parameters of molecules: BOND SmartSlide™, ANGLE SmartSlide™, DIHEDRAL SmartSlide™, INQUIRE, ADD VALENCE, and DELETE ATOM), each described below.



Inquire Mode Display

Inquire: Obtaining Geometry Information

The INQUIRE button allows you to request geometric information directly from the molecule in the [WORK AREA] window when you click on the atoms of interest.

The number of atoms selected affects the resulting display on the [WORK AREA] window, as shown in the following table.

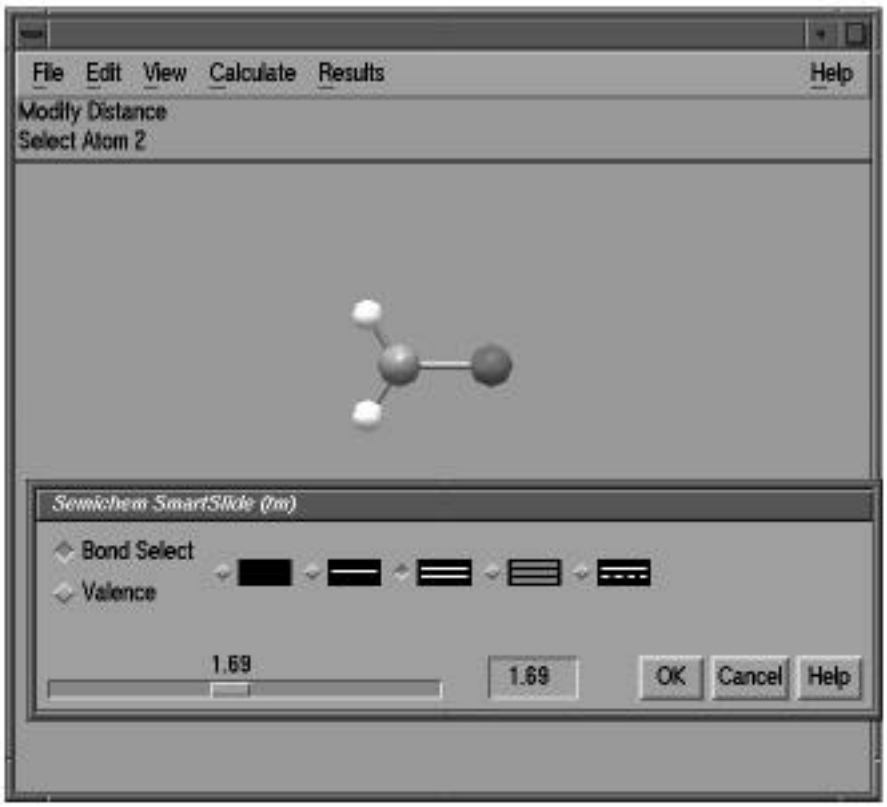
# Atoms Selected	Display
2	The bond length is displayed in the status bar (below the menus).
3	The interatomic angle is displayed.
4	The 4321 dihedral angle value is displayed.
5+	Dihedral angles are displayed for the most recent four atoms.

Hint> *To examine several structural parameters in succession, use* INQUIRE *mode. Simply click in an empty area of the window whenever you want to deselect all atoms and start a new inquiry.*

Semichem SmartSlide™ Options

Three buttons, BOND, ANGLE, and DIHEDRAL, summon the Semichem SmartSlide™ options to allow rapid and intuitive modification of geometric components.

Note: To simply examine structural parameters, we recommend that you use INQUIRE mode (described above) rather than the SmartSlide™ modes.



Bond SmartSlide™

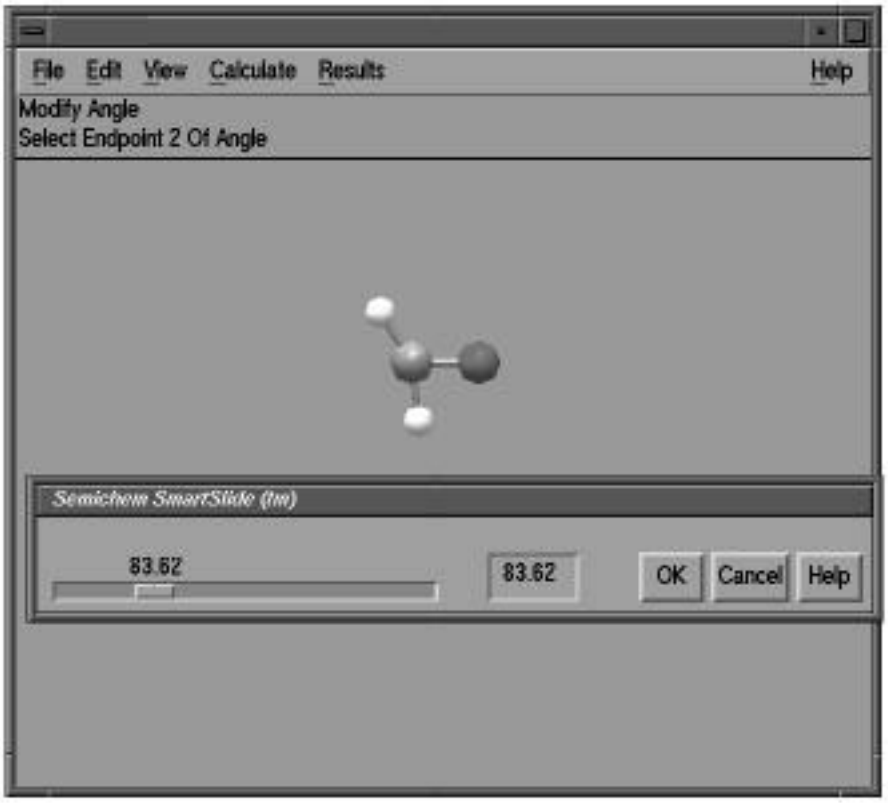
Bond: Accessing and Managing Bond Types

When you select the BOND button and highlight two atoms, the Bond SmartSlide™ is activated. The initial value is set to the distance between this pair of atoms (whether bonded or non-bonded), and the type of bond existing (if one does) between them is indicated. The SmartSlide™ provides access to all the possible bond types allowed by chemical valence rules for the particular atom type. (See "Valence" option below.)

Interatomic distance is dynamically adjusted by moving the slider along the scale. Values may also be directly typed in the text box for higher accuracy.

If you activate the "Bond Select" option, then you can change the bond type by clicking one of the bond type radio buttons without affecting the valence on the atoms from which the bonds are removed or added. (Note that this is a purely visual exercise as far as the quantum mechanics are concerned, as the methods in AMPAC and GAUSSIAN-94 do not take account of connectivity information provided by the GUI, but determine bonding from the wavefunction. It is important to retain some regularity here though, as the ***AMPAC GUI**'s* unique CLEAN function will make use of it to produce chemically meaningful structures.)

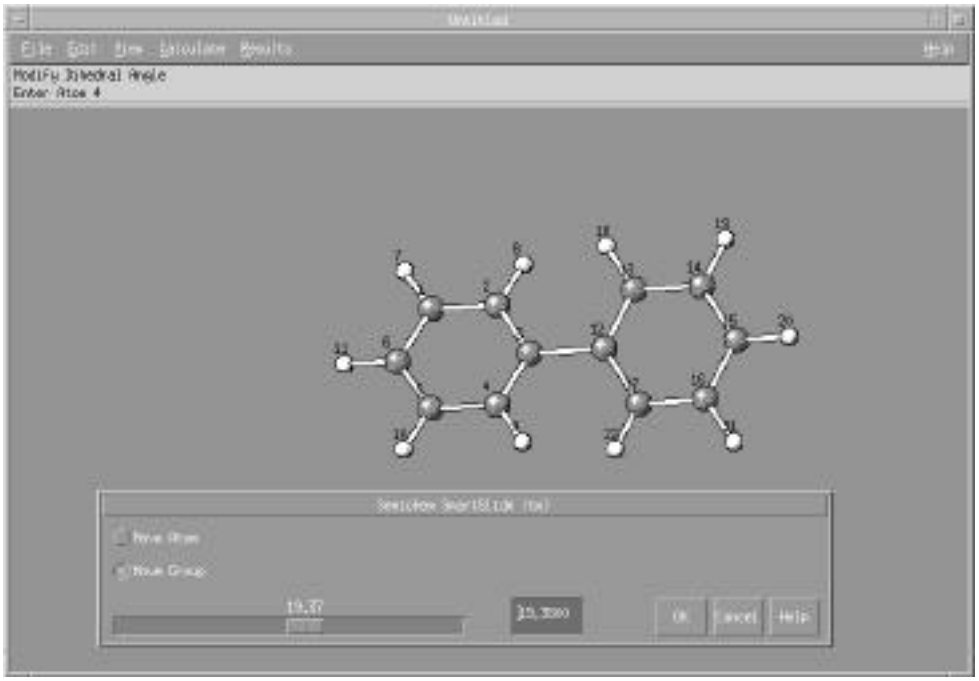
If the "Valence" option is active, valences will be adjusted, where possible, to ensure that the central atoms being changed retain the correct number of bonds. As above, the use of this function is not confined to chemically bonded pairs of atoms, Any atom pair may be selected and used here. Note that the "OK" button must be clicked before any of the changes made on the SmartSlide™ can take place.



Bond Angle SmartSlide™

Angle: Adjusting Bond Angles

Press the ANGLE button and highlight any three atoms to activate the Angle SmartSlide™. The initial value is set to the selected bond angle. You can adjust the angle dynamically by moving the slider along the scale. The first atom chosen (and any atoms dependent on that atom) is the one that moves in response to SmartSlide™ actions. Values may also be directly entered in the text box. Note that the "OK" button must be pressed before any of the changes made on the SmartSlide™ are permanent.

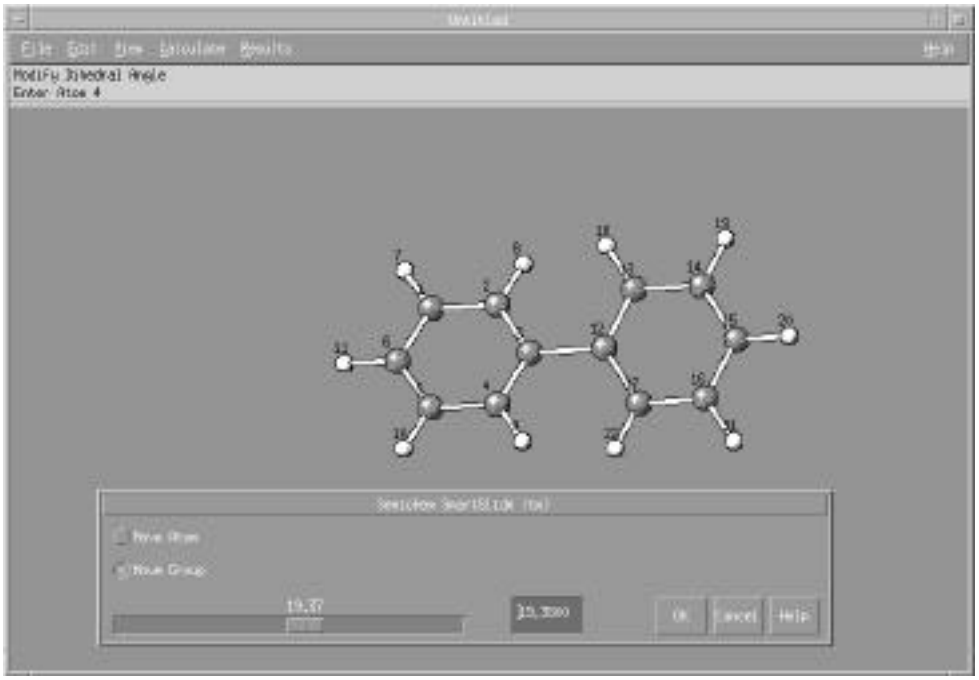


Dihedral SmartSlide™

***Dihedral*: Adjusting Dihedral Angles**

Press the DIHEDRAL button and highlight any four atoms to open the Dihedral SmartSlide™. The SmartSlide™'s initial value is set to the dihedral angle defined by the four atoms chosen.

The dihedral angle is dynamically adjusted by moving the slider along the scale. This slider has limits of –180° to 180°, giving a full 360° range of rotation. Values may also be directly entered in the text box. The first atom selected manages the motion resulting from changing the slider value.



Dihedral SmartSlide™

If you choose "Move Atom", only the first atom as noted above is moved. If "Move Group" is checked, all groups dependent on the first atom move. For example, by choosing as the first atom a hydrogen of a methyl group, the entire group can be rotated if "Move Group" is active. Note that the "OK" button must be pressed first before any of the changes made on the SmartSlide™ are permanent.

Valence Modification Functions

Valence modification functions consist of the following: ADD VALENCE and DELETE ATOM.

Add Valence: Attaching Hydrogen Atoms

Attaches additional valences (shown as hydrogen atoms) to a selected center. The new valences will be placed as far as possible from the other atoms attached to the center, and the CLEAN function (see below) will reoptimize the arrangement of bonds about the center.

Delete Atom: Removing Atoms and Single Valences

Eliminates atoms and open valences. When used, the function will eliminate the selected atom and all single valences (hydrogens) attached to it.

Other [Builder] Window Buttons

The NEW, CENTER, REBOND, CLEAN, and HELP buttons, located at the bottom of the [BUILDER]window, are described below.

New: Resetting Options and Clearing the [WORK AREA] Screen

Clears the contents of the [WORK AREA] screen and resets all the options on the dialog boxes according to the default or saved preferences (see SAVE PREFS… in the discussion of the •FILE• menu below).. Note that NEW here performs the same function as the NEW menu item on the •FILE• menu in the [WORK AREA] window. (You will be prompted to save any existing structure before NEW destroys the current information.)

Center: Optimizing the [WORK AREA]

Centers and resizes the image in the [WORK AREA] window to make the most efficient use of the workspace. This button performs the same function as the CENTER item on the •VIEWS• menu.

Rebond: Calculating and Updating Bonds

Instructs the ***AMPAC GUI*** to re-identify bonded atoms, based on a distance/nearest-neighbor algorithm. Again, note that neither AMPAC nor GAUSSIAN-94 use the bond information of the screen for calculations. This information is presented only to make it convenient for you to visualize the chemistry of the molecule. Indeed, the bonding information you set will not be retained if a calculation is performed and the bonding pattern that appears on the screen will be derived from the atomic distances. This button performs the same function as the REBOND item on the •EDIT• menu.

Clean: Adjusting Molecular Geometry

Adjusts the geometry of the molecule, based on a defined set of rules, to more closely match chemical intuition. The results are only approximations and are not intended to be perfect. Geometries may require adjustment for non-classical cases such as transition states. This button performs the same function as the CLEAN item on the •EDIT• menu.

To prevent R–OH and other groups "cleaning up" to linear structures, add a valence to the associated oxygen atoms and then change the hydrogen to a dummy atom (element X) or delete the hydrogen and leave a dangling half bond. Be sure to delete the dummy atom or half bond from the final structure after cleaning.

Using the [WORK AREA] Window Menus

Five pull-down menus (•FILE•, •EDIT•, •VIEW•, •CALCULATE•, and •RESULTS•) in the [WORK AREA] window provide options for controlling the interaction of the program with input and output files as well as visualization and calculation options. Each option in these menus is discussed below. Ellipses ("...") following an option in a pull-down menu (as in OPEN…) means that further options and controls are available when you click on it.

File Menu

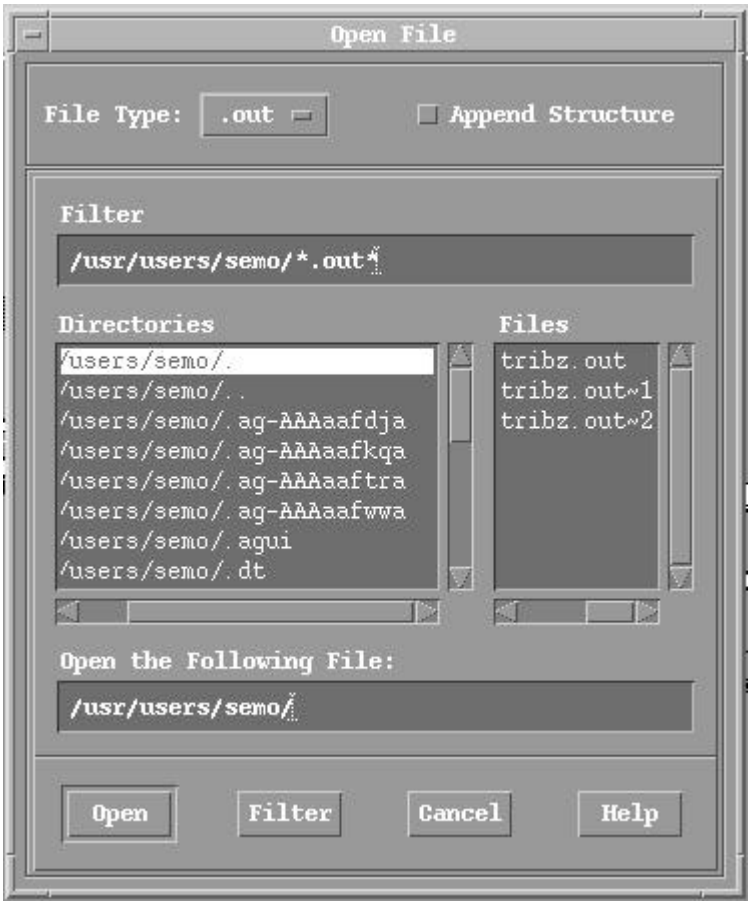
The •FILE• menu provides options for creating, modifying, and saving structures.

***New*: Resetting Options and Clearing the [WORK AREA] Screen**

Clears the contents of the screen and resets all the options on the dialog boxes according to the default or saved preferences, if you have altered these (see SAVE PREFS, below). Note that NEW here performs the same function as the NEW button on the [BUILDER]window. (You will be prompted to save any existing structure before NEW destroys the current information.)

***Open*: Opening Files**

Allows you to open files of various file formats supported by the ***AMPAC GUI***. When this option is selected, a dialog box (described below) is presented.



Using the [OPEN] Dialog Box: The "File Type" pull-down menu sets the file filter, allowing only files with particular extensions to be displayed in the browser. This means that a subset of the files in the directory with the filter string as part of their name are shown in the dialog box's "Files" list box. Available file types with brief definitions are listed below:

FILE TYPE	Description
.DAT	AMPAC data file (z-matrix + keywords)
.ARC	AMPAC summary file in plain text
.OUT	AMPAC full results file
.VIS	AMPAC summary file in binary, recomended for routine work
.COM	GAUSSIAN-94 input file (z-matrix + keywords+ Link 0)
.LOG	GAUSSIAN-94 full output file
.CHK	GAUSSIAN-94 summary file in binary
.FCHK	GAUSSIAN-94 summary file in plain text
.CUB	GAUSSIAN-94 or AMPAC surface file in plain text
.GEO	GUI file with Cartesian coordinates and symbols
.ENT	PDB file
.FRG	GUI file with Cartesian coordinates, symbols, and connectivity

Features of the [OPEN] Dialog Box:

"**File Filter**" Text Box: Only a selected set of the files in each directory are shown in the "Files" list box below according to what is present on the filter line. The filter is set automatically by the file type pop-down menu or may be entered manually by the user..

"**Append Structure**" Check Box: Select this check box to add the structure to the molecule on screen, as described in the APPEND menu item.

"**Directories**" List Box: The left scrolling list in the middle section of the dialog box is the directory listing for the present location. You can navigate the file system by going up the tree by selecting the second item on the list. You can go down into any available subdirectory within the present directory by double clicking on the directory name in the list.

"**Files**" List Box: The right-scrolling list shows the files matching the filter criteria in the current directory. You can select a file for opening by double-clicking on its name or single-clicking and pressing the OPEN button.

"**Open the Following File**" Box: Selecting a file results in the item being placed in the text box at the bottom of the dialog box, where you can also type in the explicit path to the file you want to open.

Append: Adding to Structures on Display

Opens a dialog box for adding (appending) contents of various files to the items on the screen without deleting any existing structures already in the [WORK AREA]. These structures are placed on screen and are not initially connected (*bonded*) to items already there. You can manipulate these structures independently with the mouse by holding down the Tab key (see below). The APPEND option enables you to establish a custom library of commonly-used fragments for insertion, thus speeding up calculations and making building systems easier and more intuitive.

Using the Tab Key

If two items are not bonded to one another (not connected by drawn chemical bonds on the screen), you can manipulate them individually on screen by holding down the "Tab" key and moving the cursor. When you use the "Tab" key, only the fragment nearest (almost touching) to the cursor is affected.

Hint> *If you are having trouble selecting a particular fragment on screen, make sure that the cursor is directly over one of the component atoms.*

***Save*: Saving Files**

Opens a dialog box to allow you to save various types of files. The molecule on the screen is written to a file whose format depends on the type selected from the "File Type" pop-down menu at the top of the dialog box (shown in the figure below).

Using the [SAVE] Dialog Box: When saving a file, use the "Save the Following File" text box to give the file a name. You can navigate the file system by using the browser functions (see the [OPEN] dialog box description above).

Features of the [SAVE] Dialog Box:

Append Extra COM Data: {GAUSSIAN-94 only} If enabled, this checkbox causes the ***AMPAC GUI*** to include in the saved file any additional data located at the bottom of the original input file.

Types of Format for Saving Data: Four formats are available for saving data: AMPAC, GAUSSIAN-94, GUI/Geo, and GUI/Frag, briefly described below:

AMPAC A standard AMPAC input file is prepared. This includes keywords on the keyword line(s) from the current settings on the [AMPAC] dialog box and an internal coordinate Z-matrix along with proper connectivity. Note that if the "Write Cartesians" checkbox is checked, the molecular structure is written in Cartesian coordinates whenever a file is saved until the box is unchecked.

GAUSSIAN-94 A standard GAUSSIAN-94 input file is prepared. This includes keywords on the route card from the current settings in the [G94] dialog box and an internal coordinate Z-matrix along with proper connectivity. Note that if the Write Cartesians checkbox is checked, the molecular structure is written in Cartesian coordinates whenever a file is saved until the box is unchecked.

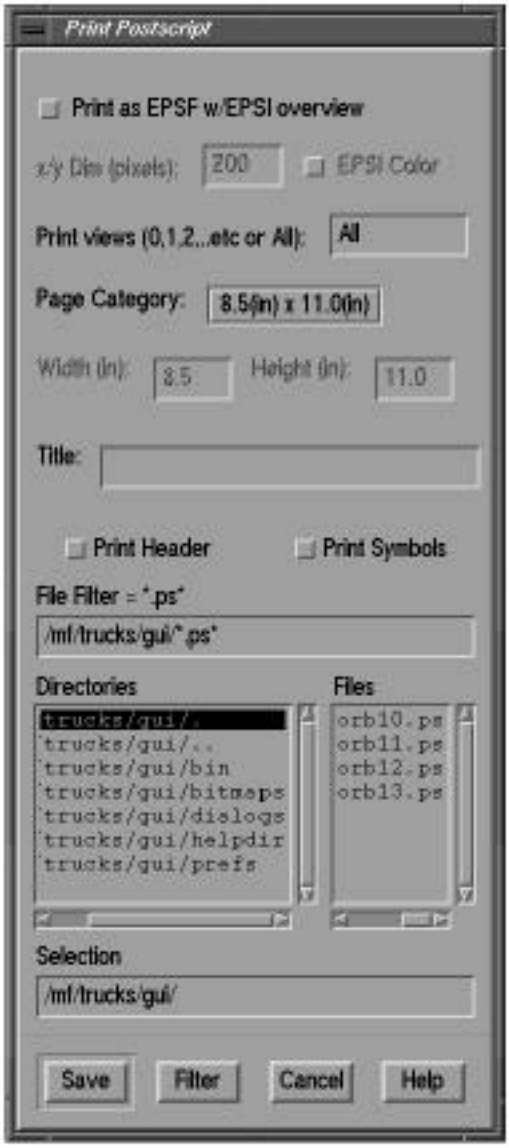
GUI/Geo A file with atomic symbols, Cartesian coordinates, and connectivity information, is written out. This format is often useful for exchanging results with other programs.

GUI/Frag A file of this type is a standard the ***AMPAC GUI*** fragment format.

***Save Prefs*: Setting New Defaults and Settings**

Saves the settings on and locations of all dialog boxes to various preferences files. These settings are used for defaults on subsequent launches of the program or the program is reset to these values when the NEW option is selected.

Caution: Make sure that all items are set the way you want them before selecting this option, as the previous values of these parameters will be changed permanently.



Print: Printing Files

Presents a dialog box that enables you to produce a PostScript® file containing a line-art representation of the image in the [W O R K A R E A]. The file can then be sent directly to a PostScript®-capable printer or exported to other graphical editing software for inclusion in documents.

The selections on this dialog box define how the file is written. The options in the dialog box are described below.

Option	Description
Print Views	Allows you to select which of the current views (open windows) will be sent to the file.
Page Category	Contains descriptions for selecting standard paper sheet sizes. The Custom option activates the *Width* and *Height* text boxes, where you may enter nonstandard sheet sizes. This information is used by the ***AMPAC GUI*** for centering and sizing the image in the file.
Title	Allows you to enter in this box text that will appear as a title in the header of the PostScript file. Note that this is not the filename of the PostScript file.
Print Header	If checked, instructs the printer to print the PostScript header information along with the contents of the selected window.
Print Symbols	If checked, instructs the printer to print the atomic symbols of each atom.
File Filter	Presents a subset of the files in a directory selected by extension.
Directories	Allows you to either move up a tree or down into any available subdirectory within the present directory.
Files	Lists the files matching the filter criteria in the present directory. Select a file by double-clicking on its name.
Selection	Displays the selected file name. Its contents are set either by editing by manually altering the text string, or selecting items from the list boxes.

Print Dialog Box Options

Exit

Closes all ***AMPAC GUI*** windows and terminates the program. Any currently-running AMPAC or GAUSSIAN-94 jobs will continue to execute.

Edit Menu

Options in •EDIT• menu allow you to perform large, global editing tasks. Each option is described below.

Undo/Redo: Reversing Editing Actions

Allows you to trace back through a series of editing actions. When the main [WORK AREA] is first opened, both of these items are dimmed, since no editing action has taken place yet. After you make the first editing change, (such as placing a molecule in the [WORK AREA]), the UNDO option becomes active and selecting it reverses the previous action. Actions may be reconstituted through the REDO option after the first UNDO. The default setting is to store 10 editing actions.

Rebond: Recomputing Bonded Atoms

Instructs the ***AMPAC GUI*** to re-identify bonded atoms, based on a distance/nearest-neighbor algorithm. Again, note that neither AMPAC nor GAUSSIAN-94 use the bond information of the screen for calculations. This information is presented only to make it convenient for you to visualize the chemistry of the molecule. Indeed, the bonding information you set will not be retained if a calculation is performed and the bonding pattern that appears on the screen will be derived from the atomic distances. This menu option performs the same function as the REBOND button on the [BUILDER]dialog box.

Clean: Adjusting Molecular Geometry

Adjusts the geometry of the molecule, based on a defined set of rules, to more closely match chemical intuition. The results are only approximations and are not intended to be perfect. Geometries may require adjustment for non-classical cases such as transition states. This menu option performs the same function as the CLEAN button on the [BUILDER]dialog box.

Clean Setup

Tunes the behavior of the CLEAN function.

View Menu

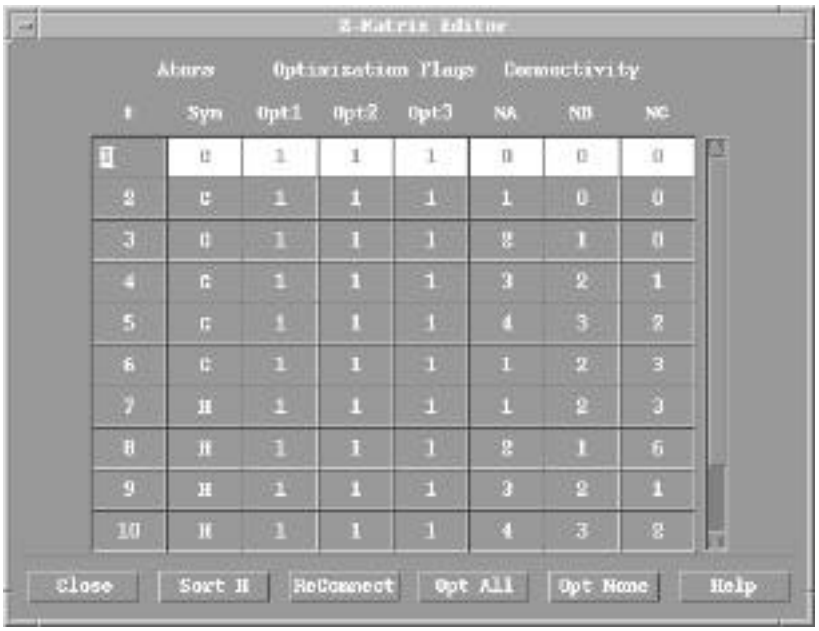
The •VIEW• menu provides options (described below) for interacting with and managing the display of molecules in the [WORK AREA] window.

Add View: Opening Additional [WORK AREA] Windows

Opens another [WORK AREA] with an independently adjustable view of the molecule.

Center: Adjusting Molecular Size to Fit the Screen

Centers and resizes the image in the [WORK AREA] window to make the most efficient use of the workspace. Note that this option has the same function as the CENTER button on the [BUILDER]dialog box.



Z-Matrix Editor Form

Z-Matrix Editor: Modifying the Structure

This dialog box facilitates your direct interaction with the geometry as the program(s) sees it in a simple and intuitive spreadsheet format. When selected, the form above is presented. Select an atom to be modified either by choosing it from the scrolling list or holding down the "Control" key on your keyboard and highlighting the atom in the [WORK AREA] window. The N_A, N_B, and N_C connectivity definition values for the selected atom are shown on the screen. (Note that the LABELS and/or NUMBERS may be used in conjunction with the Z-matrix editor to simplify selections.) Whenever changes are made, all items are recomputed to reflect the updated information.

You may carry out the following tasks in the Z-matrix editor:

- Assign partial or complete connectivity to the molecule.
- Recompute connectivity completely using a distance algorithm (REBOND button).
- Change the elemental identity in the "Sym" box
- Re-order atoms by changing the entry in the "#" box for an atom
- Turn all optimization flags on using the OPT ALL button
- Turn all optimization flags off using the OPT NONE option
- Sort all hydrogen atoms to the bottom of the list, retaining encountered order (SORT H button).

Hide/Show Builder: Displaying the [Builder] Window

Closes and reopens the [BUILDER]window. This window is displayed by default when the ***AMPAC GUI*** is launched.

Hide/Show Hydrogens: Displaying Hydrogen Atoms

Toggles the display of hydrogen atoms on and off in the [WORK AREA] window.

Hide/Show Dummy: Displaying Dummy Atoms

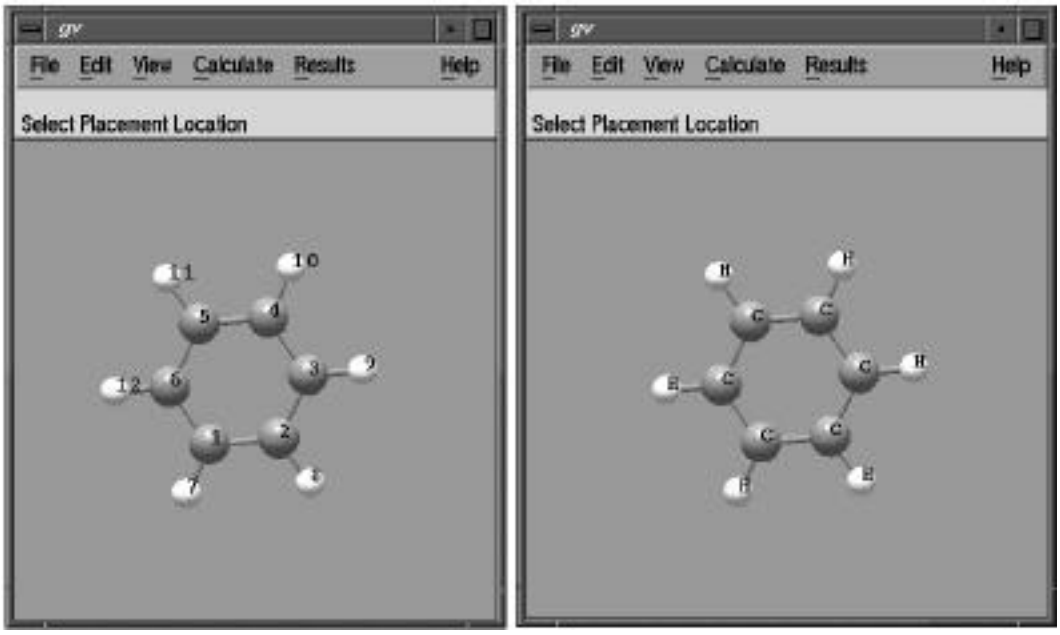
Toggles on and off the display of dummy atoms (if present). Dummy atoms are used in the construction of certain difficult geometries. See the ***AMPAC*** *User's Manual* for further explanation of the definition and use of dummy atoms.

Hide/Show Labels: Displaying Atomic Labels in the [WORK AREA] Window

Writes atomic labels on top of the atoms displayed in the [WORK AREA] that represent the sequence number of the atom in the list of atoms. It may be used with or without SYMBOLS (see below).

Hide/Show Symbols: Displaying Element Symbols

Displays the chemical symbol for each atom in the [WORK AREA] window. It may be used with or without LABELS (see above).



Show Labels Display (left) and Show Symbols Display (right)

Display Format: Selecting the Display Format

Presents a dialog box for selecting the format of the display in the [WORK AREA] window. The dialog box options differ, depending on whether the graphical environment your system is X-Windows or OpenGL. Descriptions of both formats follow.

X-Windows Systems

For X-Windows systems, options in the molecular display format dialog box (at left) control how the molecule appears in either of the following instances:

In Motion: When the molecule is in motion.

Stationary: When the molecule is static.

The radio buttons in this dialog box allows you to select the visual format model (described in the following table) on which the image on the [WORK AREA] window is based.

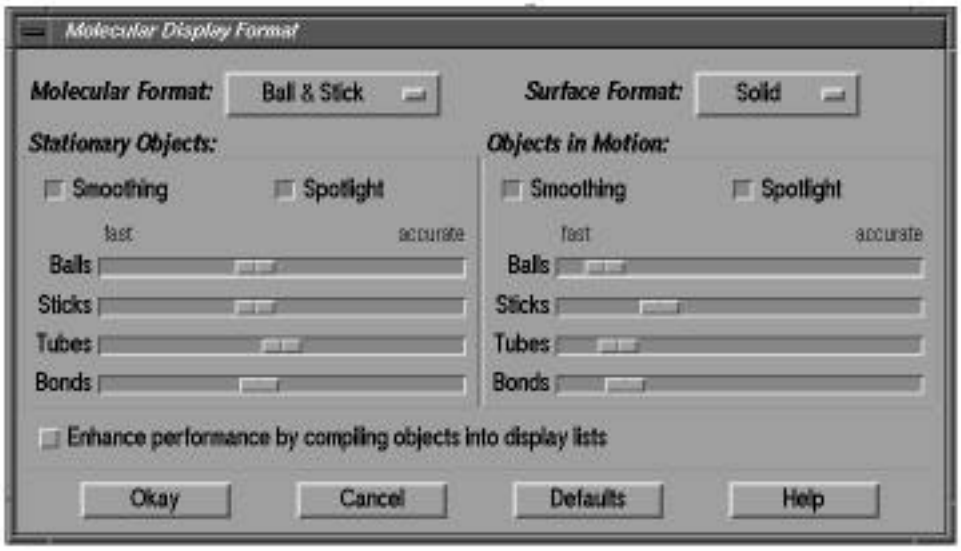
Molecular Model	Description
Wireframe	Shows only connectivity and bond types; does not show any atoms. This mode allows you to see the bond types assigned by the ***AMPAC GUI***. It is the simplest mode and is preferred for slower workstations
Ball & Stick	Displays atoms and connectivity with some perspective information.
Shaded	Allows you to request perspective shading of atoms. This mode shows atoms and connectivity with shadows added, to best represent perspective.

X-Mode Systems Molecular Models

Hint> *It is often convenient to keep "Static Display" in "Shaded" mode and "Motion Display" in "Wireframe" mode so that any small mouse movement will bring the full bond description to light.*

OpenGL Systems

OpenGL Mode options in the molecular display format dialog box govern the molecule's appearance both when it is being moved in the [WORK AREA] window by mouse action, and when it is still. It is often useful to use an "Accurate" mode for "Stationary Objects" and a "Fast" mode for "Objects in Motion".



Molecular Display Format Dialog Box (OpenGL Format)

Positioning the sliders in the dialog box toward the "Accurate" end of the various scales produces more aesthetically appealing graphics but requires more computational effort and slows down response of the graphic image on screen.

The molecular display format dialog box allows you to select the type of visual model on which the image in the [WORK AREA] is based. Options in this dialog box are described in the following table:

Molecular Model	Description
Ball & Stick	Molecule appears as a ball and stick model, with all types of bonds represented by single sticks.
Ball & Bond Type	Molecule appears as a ball and stick model with single bonds represented by single sticks, and multiple bonds represented by multiple sticks, or in the case of aromatic systems, by dotted lines.
Tube	Molecule appears as a tube model with no indication as to bond type. Atom types are indicated by color bands on the tubes.

OpenGL Systems Molecular Models

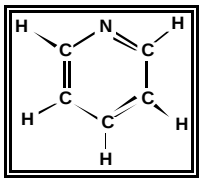
Surface Format

The "Surface Format" pull-down menu allows you to select the appearance of surfaces generated by the ***AMPAC GUI***. (Only "Mesh" is available in X-Windows for surface display.) Note that the surfaces are superimposed onto the molecular framework chosen above.

Surface	Description
Solid	Surface appears as solid lobes.
Mesh	Surface appears as a mesh, allowing the user to display both the surface and the underlying atoms.
Translucent	Surface appears smooth but translucent, and underlying atoms are visible.

Surface Format Options

Molecule Building Examples



Building Pyridine: Using Untyped Atoms

1. Start a new file by selecting the NEW option from the •FILE• menu in the [WORK AREA] window. ⇒

2. Select RINGS on the [BUILDER]window. ⇒

3. Click on the ACTIVE FRAGMENT window. ⇒ Select benzene from the ring fragments. ⇒

4. Return to the [WORK AREA] window. ⇒ Click once: benzene displays. ⇒

5. Click on ELEMENT on the [BUILDER]window. ⇒Click on nitrogen.⇒

6. Click on the ACTIVE FRAGMENT display. ⇒ Click on the Nitrogen atom. ⇒

7. In the [WORK AREA] window, click on the carbon atom you want to change to nitrogen. ⇒

Hint>

In this example you have not selected one of the nitrogen hybridization fragments, but the untyped atom. If you selected the aromatic nitrogen fragment, you could replace a ring carbon with an aromatic nitrogen. This is different from using the N-atom fragment in that the extra hydrogen atom is automatically removed and the C-N bonds are adjusted to a more reasonable value.

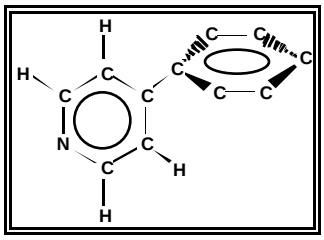
8. Select the DELETE ATOM button from the [BUILDER]window. ⇒ On the [WORK AREA] window, delete the hydrogen attached to the nitrogen by clicking on it. ⇒

9. Click on the CLEAN button to adjust the structure.

Hint>

You will often want to rebond before cleaning. Clean uses a variation of atom typing for guidance in optimization.

Pyridine is now complete.



Building Phenylpyridine: Setting the Angle Between Rings

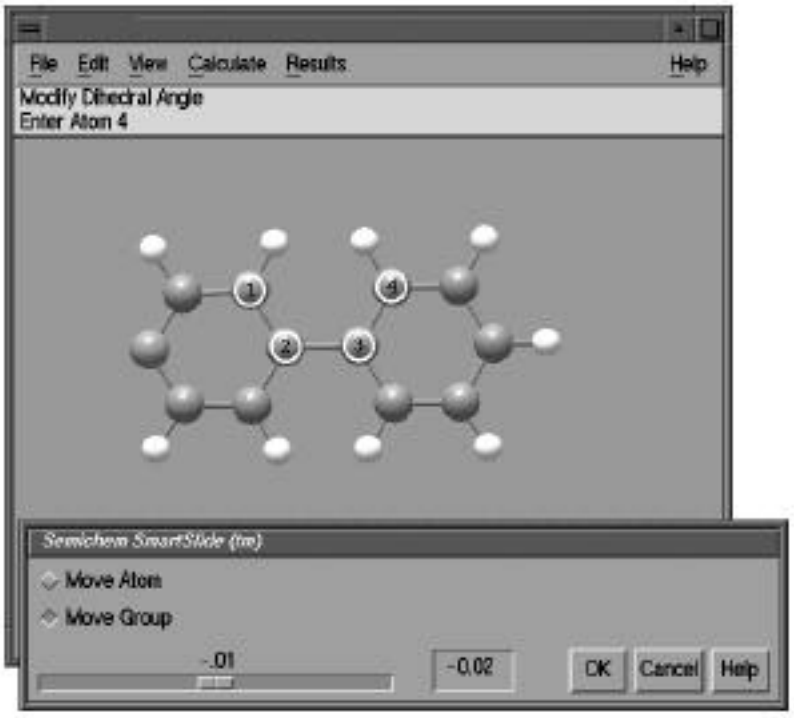
This example shows how to build Phenylpyridine based on an existing file, in this case the pyridine molecule you built in the last example..

1. Click on RINGS on the [BUILDER]window. ⇒ Be sure that the benzene ring is selected (is shown in the ACTIVE FRAGMENT window). ⇒

2. Click on the hydrogen atom located on the carbon atom opposite the nitrogen atom on the molecule in the [WORK AREA] window. ⇒ A second ring is displayed on the screen. ⇒

3. Select the DIHEDRAL button on the [BUILDER]window. ⇒

4. Select atoms between the two rings, as shown in the following figure. ⇒

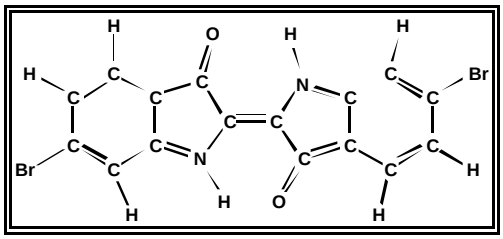


Modifying the Dihedral Angle

5. (*Note:* Make sure that the "Move Group" item is chosen to allow rotation of the entire pendant ring. Otherwise, only the first atom selected will move ("Move Atom" mode).) Move the slider to create a dihedral until the rings are perpendicular to each other (value at 90°). ⇒

6. Click on the OK button.

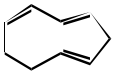
Phenylpyridine is now complete.



Building Tyrian Purple Dye: Appending a Structure

The following is an example of how a Tyrian purple dye (6,6'-dibromoindigo) is constructed in the ***AMPAC GUI***:

1. Select NEW from the •FILE• menu. ⇒



2. Select the fused 5 and 6 carbon rings on the [BUILDER]window from the RINGS form (see illustration at left). ⇒ Click on the [WORK AREA] window to place the fragment.

3. Select oxygen from ELEMENT and change the appropriate hydrogen atom in the five-membered ring to an oxygen by clicking on it. ⇒

4. Change the carbon atom opposite the newly placed oxygen to nitrogen using one of the methods illustrated in the first example. ⇒

5. Change the hydrogen atom on the outermost carbon atom in the six-membered ring (on the same side as the nitrogen) to bromine in a similar manner. ⇒

6. Select CLEAN on the [BUILDER]window. Do <u>not</u> rebond. ⇒ Then save the file by choosing SAVE... from the •FILE• menu. ⇒

7. APPEND the file you just saved to the display onto the [WORK AREA] window. ⇒

8. Rotate and move the second ring so that the two carbon atoms to be bonded are close together, and the two fragments are oriented properly with respect to one another. ⇒

Hint>

To affect only <u>one</u> of the two unbonded fragments, hold down the "Tab" key while dragging the mouse.

Using a second window is often helpful when performing complex positioning operations. Use the ADD VIEW *option on the* •EDIT• *menu to create one.*

9. Delete the hydrogen atoms on the two carbon atoms to be bonded. ⇒

10. Select BOND on the [BUILDER]window. ⇒ Create a single bond between the two carbon atoms by selecting the single-bond radio button.⇒

Hint>

Alternatively, choose the BOND item on the [BUILDER]window, check the "Valence" box, select the two carbons to be bonded and choose the single-bond radio button. The two extra hydrogens will be automatically eliminated to preserve proper valence on the carbons.

11. Click on CLEAN.

The 6,6'-dibromoindigo molecule is now complete.

3 Setting Up and Running AMPAC and GAUSSIAN-94 Jobs

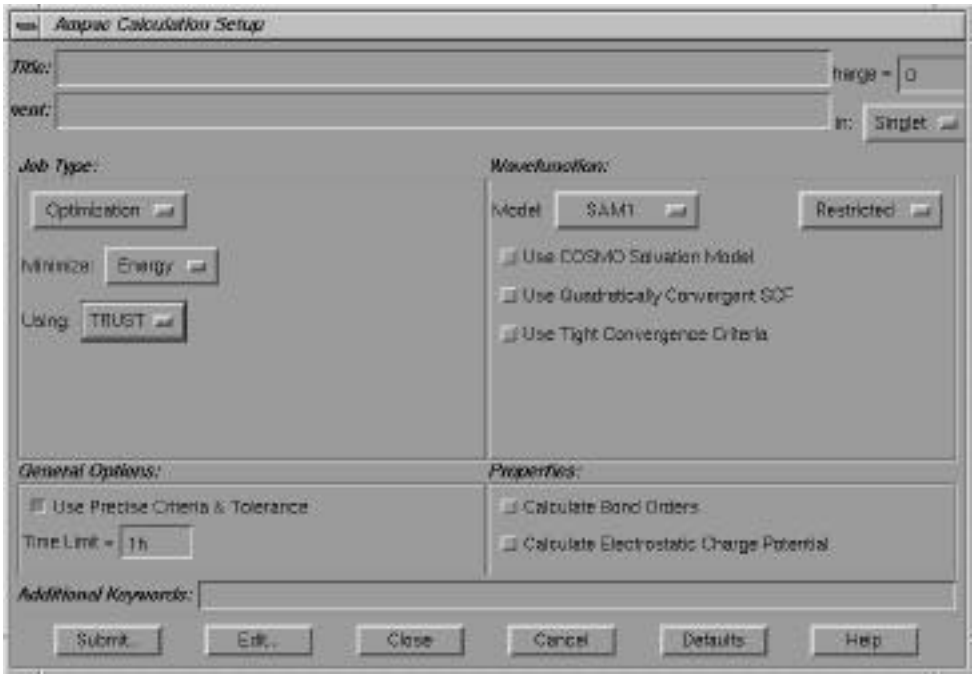
The ***AMPAC GUI*** provides a convenient interface for setting up, submitting, and managing AMPAC and GAUSSIAN-94 jobs through the •CALCULATE• menu and its three dialog boxes, AMPAC, G94, and CURRENT JOBS. Through these dialog boxes, you can easily create AMPAC or GAUSSIAN-94 input files, set options for AMPAC and GAUSSIAN-94 calculations, submit jobs to the computer, and view current jobs without leaving the ***AMPAC GUI***. The first section of this chapter describes procedures for creating and running AMPAC and GAUSSIAN-94 files by using options available through the ***AMPAC GUI*** •CALCULATE• menu. The second section of this chapter describes options available through the CURRENT JOBS menu, which allow you to manage jobs started by the ***AMPAC GUI*** that are currently running in the background.

AMPAC Option: Creating an Input File

The first step in producing an AMPAC input file is to build the desired molecule using the various construction functions available in the interface. The bond lengths, bond angles, and dihedral angles specified in the [BUILDER]window will be used by the ***AMPAC GUI*** to write an input file for the calculation.

Select the SAVE... option under the •FILE• menu, choose the "AMPAC" file type (default) from the pop-down menu, enter a name, and click OK to create the input file.

The Z-matrix and the options selected (or the defaults) on the [AMPAC] dialog box (below) comprise the items written to the AMPAC input file.



[AMPAC] Dialog Box

The [AMPAC] Calculation Setup dialog box contains several sections, described individually below.

"Title" Section

Contains a description of the job. Type your description into the text box. It will be included verbatim on the second line of the input file.

"Comment" Section

Contains further information to identify the calculation. Type your description into the text box. It will be included verbatim on the third line of the input file.

"Job Type" Section

Allows you to select the type of calculation to be carried out. The default is for an Optimization. The following table shows this section's job types and the available options associated with them.

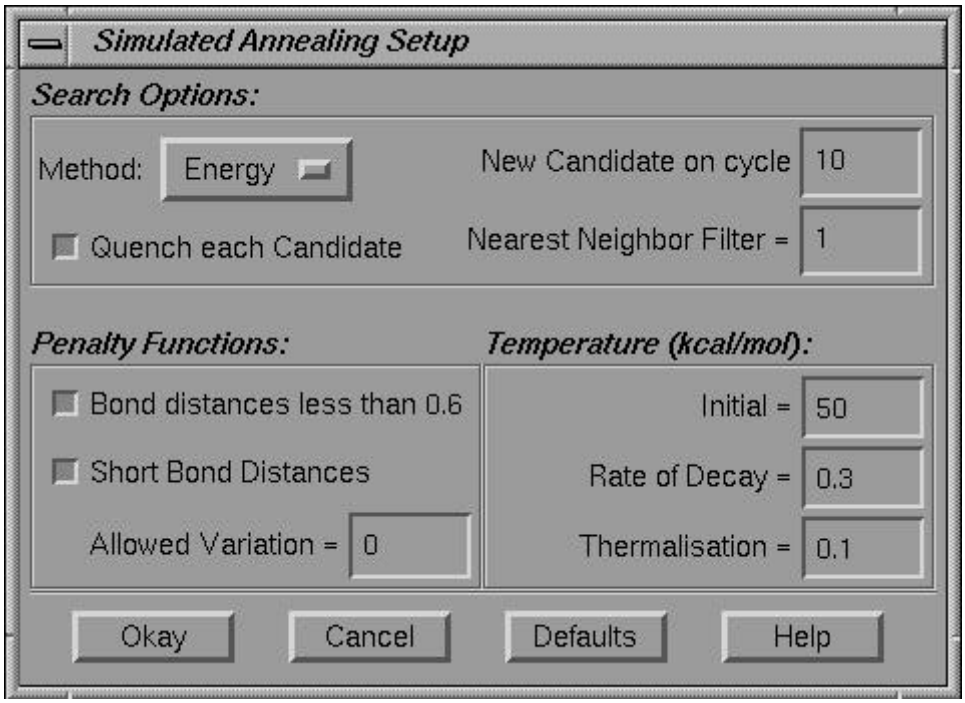
Selected Job Type	Selected Options	Defaults	Corresponding AMPAC Keyword & Options
Energy	*none*		1SCF
Optimization	*Minimize* = Energy *Using* = TRUST		TRUSTE
	Minimize = Energy *Using* = EF		EF
	Minimize = Gradient *Using* = TRUST		TRUSTG
	Minimize = Gradient *Using* = EF		TS
Frequency	Calculate Thermodynamic Properties	off	*On:* THERMO
IRC	*none*		IRC
	forward		IRC TV=n
	reverse		IRC TV=–n
Reaction Coordinate			
Simulated Annealing			

Selected Job Types and Available Options

Note that the IRC option will call for a computation of vibrational modes and will follow the nth mode as indicated here. This is useful for examining the reactants and products connected by a particular transition state. It is likely best to perform an LTRD or FORCE calculation prior to invoking IRC so that the actual vibrational modes can be examined.

The REACTION COORDINATE option requires the user to assign a single coordinate in the z-matrix as the reaction coordinate to be used for the calculation. Clicking the Z-MATRIX EDITOR button (appears when this job type is chosen) will present the z-matrix in editable form. The user must choose one of the coordinate and set the optimization flag to "-1". You may then enter the number of steps you wish to take and the interval of each step in the text boxes.

The SIMULATED ANNEALING job type has an entire dialog box governing the options associated with it. You may access this dialog box by selecting the OPTIONS button that appears when this job type is selected. The following is an explanation of the dialog box and settings corresponding to its options.



[Simulated Annealing] Dialog Box

Annealing searches may be done either for energy minima or gradient minima. See Chapter 9 of the ***AMPAC*** *Users Manual* for a more complete description of the keywords. The options on this dialog box correspond to particular annealing keywords as noted below:

	Selected Options	Defaults	Corresponding AMPAC Keyword & Options
Locate	Energy Minima		ANNE
	Gradient Minima		MANN
No Quenching		*off*	NOQU
New Candidate every...	*=n*	10	NCHECK=n
Nearest Neighbor....	*=n.nn*	1.00	FILTER=n.nn
Penalty Functions	<0.6 Bond Distances	*on*	PEN1
	Short Bond Distances	*on*	PEN2
	Allowed Variation	0.00	TOL=n.nn
Temperature	Initial=n.nn	50.00	TEMP=n.nn
	Decay=n.nn	0.30	TLAW-0.30
	Thermalization=n.nn	0.10	SIGMA=0.10

Simulated Annealing Options

"Wavefunction" Section

Selects the semiempirical model and the type of wavefunction to be used in the calculation.

Selected Wavefunction	Selected Options	Defaults	Corresponding AMPAC Keyword & Options
Model	AM1	AM1	AM1
	SAM1		SAM1
	MNDO/d		MNDOD
	MNDO		MNDO
	MINDO/3		MINDO
	MNDOC		MNDOC
	PM3		PM3
	SM1-AM1		SM1 AM1 DERINU
	SM2-AM1		SM2 AM1 DERINU
	SM3-PM3		SM3 PM3 DERINU
Type	Restricted	Restricted	RHF
	Unrestricted		UHF
	C.I.=n	2	C.I.=n MECI
Use COSMO...	COSMO=x.xx	off	COSMO=79.6
Use Quadr....		off	QCSCF
Use Tight...		off	SCFCRT=0

Selected Wavefunctions and Available Options

When C.I. (configuration interaction) is requested, a text box is added to this section that has a default value of C.I.=2 in place. If used as is, this would call for a CI calculation using the HOMO and When C.I. (configuration interaction(is requested, a text box is added to this section that has a default value of C.I.=2 in place. If used as is, this specification would call for a CI calculation using the HOMO and LUMO only. You may change this value, but be take care, in that unless you are familiar with the arrangement of the MOs (by having done an AMPAC calculation using VECTORS), the default calculation may fail for a number of reasons. The CI module in AMPAC is very flexible and has many options. See the ***AMPAC*** *User's Manual* for a more complete description.

When a COSMO calculation is requested, an additional text box is also added to this section. It initially contains the dielectric constant for water, the default solvent. You may enter another value here for a different solvent of your choice.

"General Options" Section

Sets options for the entire calculation.

Selected General Option	Defaults	Corresponding AMPAC Keyword & Options
Bond Orders	*on*	BONDS
Time	*1 hour*	T=1h
Accurate Calc...	*on*	PRECISE
Electrostatic Charges	*off*	ESP

General Options

The PRECISE option listed above should be used for most calculations. It may need to be disabled to achieve convergence when very large molecules (over 100 atoms) are being studied. The use of PRECISE subjects all phases to more stringent termination criteria, making the results more reliable.

"Charge" and "Spin" Section

You can use the input box and pull-down menu located in the upper right-hand corner of the dialog box to specify Charge and Spin multiplicity.

"Additional Keywords" Section

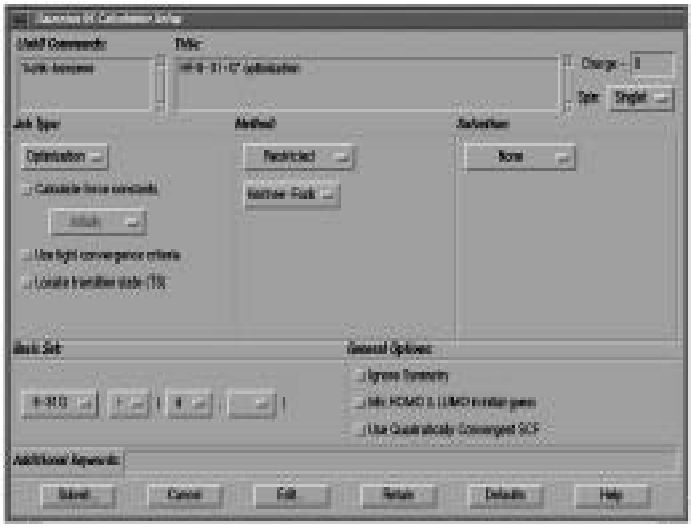
You can directly enter keywords to be appended to the AMPAC keyword line(s) in this text box to control AMPAC options not yet implemented in the interface.

Dialog Box Buttons

The following table describes the buttons on the [AMPAC] Calculation Setup dialog box.

Button	Description AMPAC
Submit	Starts an AMPAC calculation using the current input file. The input file is not available for submission until the file has been saved.
Cancel	Closes the dialog box and returns all selections to their default values.
Edit	Allows direct access to the input file within a text editor. The input file is not available for editing until the file has been saved.
Close	Closes the dialog box. Current selections are retained but the input file is not created until the file has been saved.
Defaults	Returns all items to their default values.
Help	Provides on-line help for this dialog box.

[AMPAC] Dialog Box Button Functions



GAUSSIAN-94 Calculation Setup Dialog Box

G94 Option

Note: Certain support programs installed with GAUSSIAN-94 are needed for the ***AMPAC GUI*** to be fully integrated with GAUSSIAN-94. Please be sure that you have Revision E or later of the Gaussian Utilities or contact Gaussian Inc. for an update.

The first step in producing a GAUSSIAN-94 input file is to build the desired molecule. The bond lengths, bond angles, and dihedral angles specified in the [BUILDER]window will be used by the ***AMPAC GUI*** to write a Z-matrix for the calculation.

Select the SAVE... option under the •FILE• menu, choose the "Gaussian" file type from the pop-down menu, enter a name, and click OK to create the input file. The Z-matrix corresponding to the molecule in the [WORK AREA] and the options selected (or their defaults) on this dialog box will comprise the items included in the GAUSSIAN-94 input file.

The [G94] setup dialog box contains several sections, each described below.

"Title" Section

Contains a description of the job. Type your description into the text box. It will be included verbatim in the input file.

"Job Type" Section

Allows you to select the type of calculation to be carried out. The default is for a single-point calculation. The following table shows this section's job types and the options available for each of them.

Selected Job Type	Selected Options	Defaults	Corresponding G94 Keyword & Options
Energy	Current Method	default	*none*
	G1		G1
	G2		G2
	CBS-4		CBS-4
	CBS-Q		CBS-Q
Optimization	*none*		OPT
	Calculate force constants: initially	Off	OPT = CalcFC
	Calculate force constants: at every point	Off	OPT = CalcAll
	Use tight convergence criteria	Off	OPT = Tight
	Locate transition state (TS)	Off	OPT = TS
Frequency	Compute Raman intensities	checked	Freq (*if checked)* Freq=NoRaman (*if unchecked)*
OPT + Freq	Compute Raman intensities	checked	Opt Freq
	All other Opt *and* Freq *options are available as above.*		
IRC	*none*		IRC
	Follow IRC one way: forward	Off	IRC = Forward
	Follow IRC one way: reverse	Off	IRC = Reverse
	Compute more points, N=___	Off	IRC = (Max Points = *N*)
	Calculate initial force constants	Off	IRC = CalcFC
Scan	Normal	default	Scan
	Relaxed		OPT = (Scan, AddRedundant)
Stability	*none*		Stable
	Reoptimize the wavefunction	Off	Stable=Opt
NMR	*none*		NMR

"Method" Section

Allows the selection of the quantum mechanical method to be used in a calculation. The default method is Hartree-Fock.

Selected Method	Selected Option	Defaults	Corresponding G94 Keyword & Options
Hartree-Fock	*none*		HF
B3LYP	*none*		B3LYP
B3PW91	*none*		B3PW91
MP2	*none*		MP2
	Include all electrons	Off	MP2(Full)
MP4	Exclude Triples	On	MP4(SDQ)
	Include Triples	Off	MP4
	Include all electrons	Off	MP4(Full)
QCISD	Exclude Triples	On	QCISD
	Include QCI Triples	Off	QCISD(T)
	Include QCI & MP4 Triples	Off	QCISD(T,E4T)
	Include all electrons	Off	QCISD(Full)
CASSCF	Number of Electrons=___ (*sets n—required*)	2	CASSCF(*n*,*m*)
	Number of Orbitals=___ (*sets m—required*)	2	CASSCF(*n*,*m*)
	RFO Quadratic Step	Off	CASSCF(*n*,*m*,RFO)
Excited State	Singlet States Only	On	CIS(Singlets)
	Triplet States Only	Off	CIS(Triplets)
	Singlet & Triplet States	Off	CIS(50-50)
	Default	Off	CIS
	Solve for more states, N=___	3	CIS=(NStates=*N*)
	Solve for specific state, Root=___	1	CIS=(NRoot=*Root*)

Selected Methods and Available Options

The following choices apply to all methods except CASSCF:

Selection	Keyword Prefix G94
Restricted	R
Unrestricted	U
Restricted-Open	RO

Closed/Open Shell Options

"Solvation" Section

The Solvation section provides choices of models to perform calculations in the presence of a solvent. The models and related additional keywords are described beginning on page 151 of the *GAUSSIAN-94 User's Reference*.

Selected Model	Input Area	Value G94
None (*Gas Phase*)	*none*	
Dipole & Sphere	Dielectric Constant	Solvent ε value
	Solute Radius (A)	Cavity radius (a_0)
PCM model	Dielectric Constant	Solvent ε value
	Npts/Sphere	# Points/Atomic Sphere
I-PCM model	Dielectric Constant	Solvent ε value
	IsoValue (optional)	Isodensity surface contour
SCI-PCM model	Dielectric Constant	Solvent ε value
	IsoValue (optional)	Isodensity surface contour

Required Parameters for Solvation Models

Note: Only the solvation options available with the currently selected method are enabled.

"General Options" Section

The following table outlines the options available in the General Options section of the GAUSSIAN-94 Calculation Setup dialog box:

Option	Default	Corresponding G94 Keyword (If Checked)
Ignore Symmetry	Off	NoSymm
Mix HOMO & LUMO in initial guess	Off	Guess=Mix
Use Quadratically Convergent SCF	Off	SCF=QC

General Options

"Basis Set" Section
Allows the selection of the quantum mechanical model to be used in the calculation. Polarization functions (* or **) and Diffuse functions (+ or ++) may be added to the basis set.

Select the blank item at the top of the basis set menu to select a basis set other than those constructable via the controls in this area. You may enter any basis set keyword in the Additional Keywords area.

"Charge" and "Spin" Section
You can use the input box and pull-down menu located in the upper right-hand corner of the dialog box to specify Charge and Spin multiplicity.

"Additional Keywords" Section
You can type in keywords to be added to the GAUSSIAN-94 route section in the lower section of the [G94] dialog box.

Note: This area is designed only for adding keywords to the route section. Use the EDIT button for creating more complex input files.

"Link 0" Commands Section
Used for entering Link 0 commands such as "%Chk". Note that if the %chk default value is left as noted, the ***AMPAC GUI*** will write "%chk=root.CHK" in the saved GAUSSIAN-94 file, where "root" is the saved file's root name.

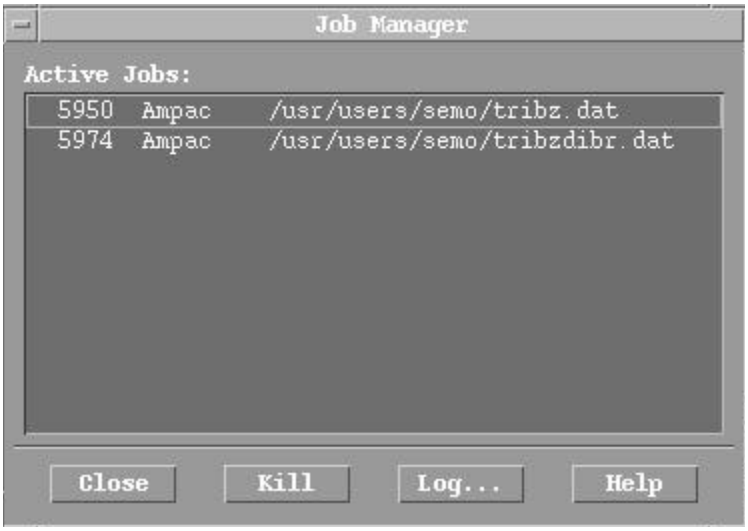
Dialog Box Buttons
The following table describes the buttons on the [G94] dialog box.

Button	Description G94
Submit	Starts a GAUSSIAN-94 calculation using the current input file. The input file is not available for submission until the file has been saved.
Cancel	Closes the dialog box and returns all selections to their default values.
Edit	Allows direct access to the input file within a text editor. The input file is not available for editing until the file has been saved.
Retain	Closes the dialog box. Current selections are retained but the input file is not created until the file has been saved.
Defaults	Returns all items to their default values.
Help	Provides on-line help for this dialog box.

[G94] Dialog Box Button Functions

Controlling Active Jobs in the *AMPAC GUI*

This window displays all the jobs started by the ***AMPAC GUI*** that are currently running. Note that only jobs started during the current session of the ***AMPAC GUI*** can be displayed.



Active Jobs Display

Clicking on the LOG button displays the current job log containing system messages associated with the execution of all job processes begun during this *AMPAC GUI* session. Individual jobs may be aborted by selecting the job to be terminated from the scrolling list and clicking on the KILL button. Examples of jobs that will be shown here are AMPAC jobs submitted from the [AMPAC] dialog box, GAUSSIAN-94 jobs submitted from the [G94] dialog box, edit sessions, and/or cubegen processes for building surfaces for display.

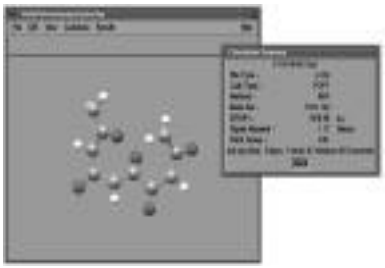
4 Visualizing Results from AMPAC and GAUSSIAN-94

Results Menu

The •RESULTS• menu opens a series of dialog boxes that allow you to examine the results of calculations from AMPAC and/or GAUSSIAN-94 output files. If particular information is not present in the file that was read into the *AMPAC GUI,* the item is dimmed in the menu.

"Summary": Getting the Summary of Calculation Results

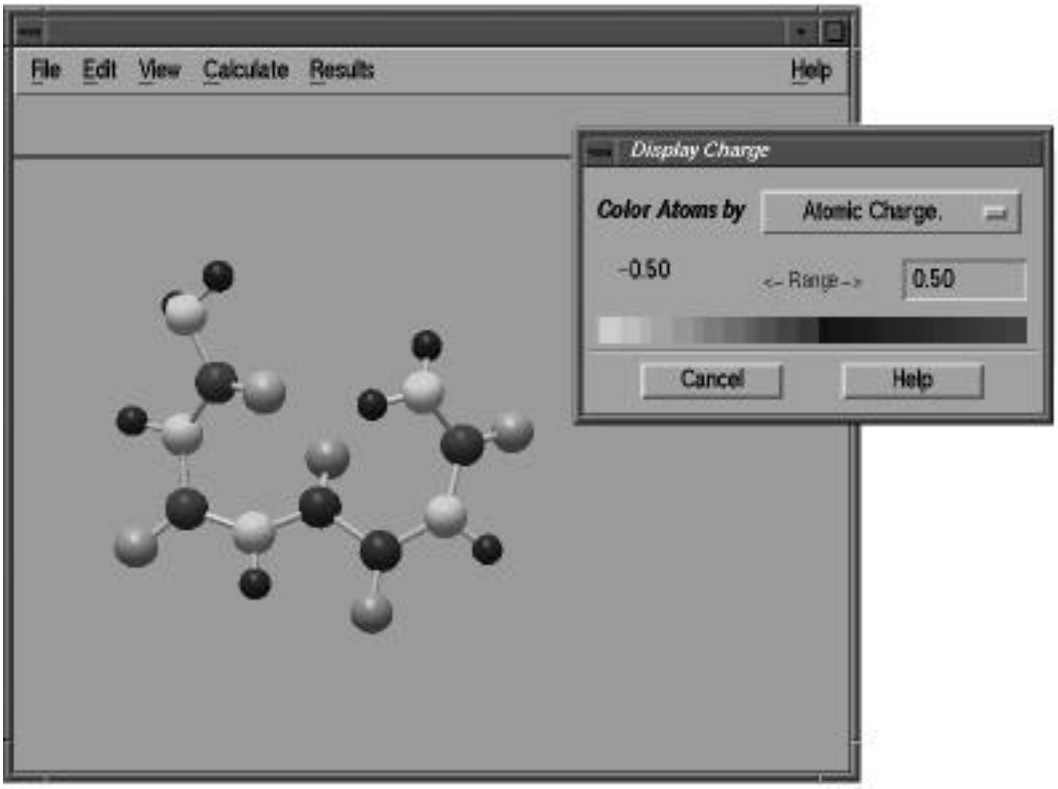
The summary data dialog box reflecting the results of the calculation become available when an .ARC or .OUT (from AMPAC) or a .LOG, .CHK, or .FCHK (from GAUSSIAN-94) file is opened from the OPEN... option on the •FILE• menu.



Calculation [Summary] Display

"Charges": Displaying Atomic Charges Computed in AMPAC and GAUSSIAN-94

This dialog box manages the display of partial charge density as computed by various methods in AMPAC or GAUSSIAN-94. Displays are available for Coulson (default) and ESP (if requested) charges for AMPAC. For GAUSSIAN-94, Mulliken (default) and ESP) charges (if requested) are the charge methods currently supported.



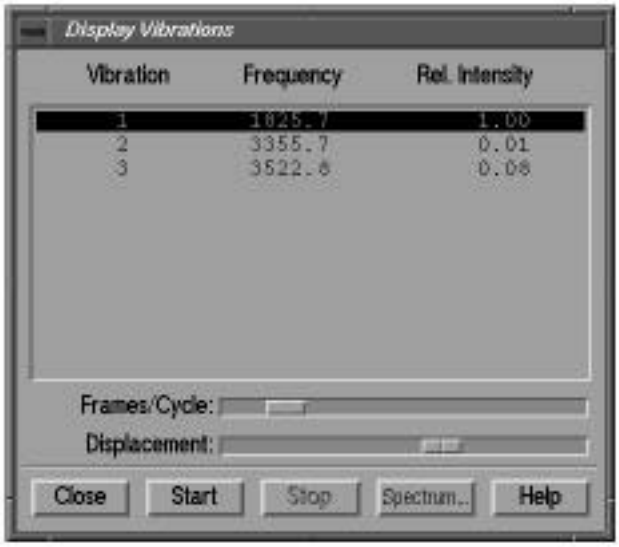
Atomic Charges Display

The pop-down menu indicates the types of display available, depending upon the information from the file that was opened. Note that the *Atom Type* selection displays the default atomic colors of the ***AMPAC GUI***.

The color spectrum for charge is set by reading the maximum charge computed for the molecule and setting the range to match the charge. The range can also be adjusted manually by entering a value into the box; note that the positive and negative values will be adjusted to the same magnitude.

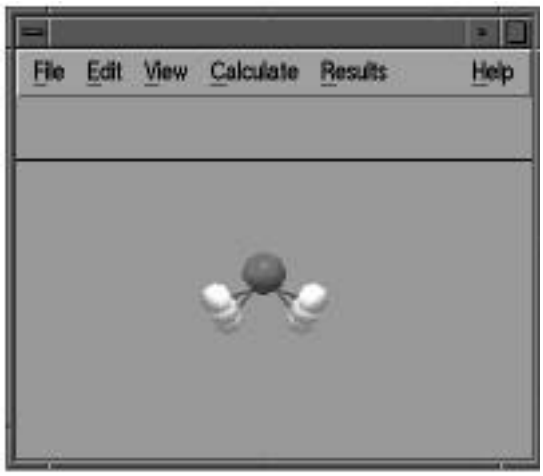
"Vibrations": Displaying Vibrational Modes and Line Spectra

Allows calculated vibrational data to be displayed as dynamic screen motions, based on information from a frequency calculation. The following is an example of a window displayed when you select the VIBRATIONS option:



Vibrations Option Dialog Box

The Display Vibration dialog box shows which vibration is currently selected for dynamic display. You can start this display by selecting the *Start* button, and halt it by clicking STOP. The molecule cycles through displacements along the motions corresponding to the vibration selected.

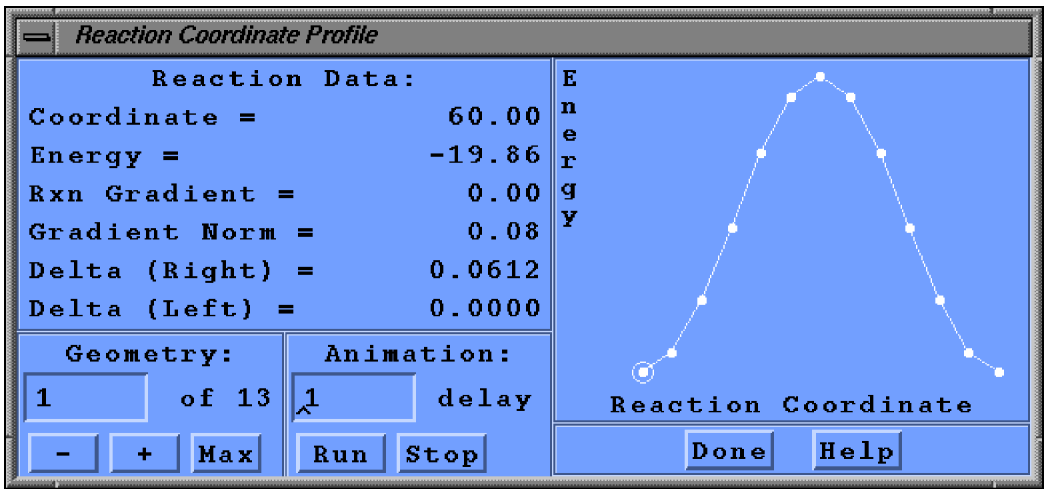


You can select other modes by typing a number in the "Display Vibration" text box, or pointing to the vibration on the scrolling list. This may be done dynamically, that is, a new vibration is selected before the previous one is halted. You can also rotate and move the vibrating molecule or view the vibration in multiple windows from different perspectives using ADD VIEW from the •VIEWS• menu. Note that only one vibration may be animated at a time.

The two slide bars at the bottom of the screen adjust the speed and magnitude of the motion. The SPECTRUM button presents AMPAC's or GAUSSIAN-94's estimate of the vibrational spectrum in line format. Note that the intensity values are relative to the highest value in the present set, and bear no precise relationship to experimental band intensities. There are significant approximations made in the computation of these intensities, and they should be interpreted with care.

"Reaction Profile....."

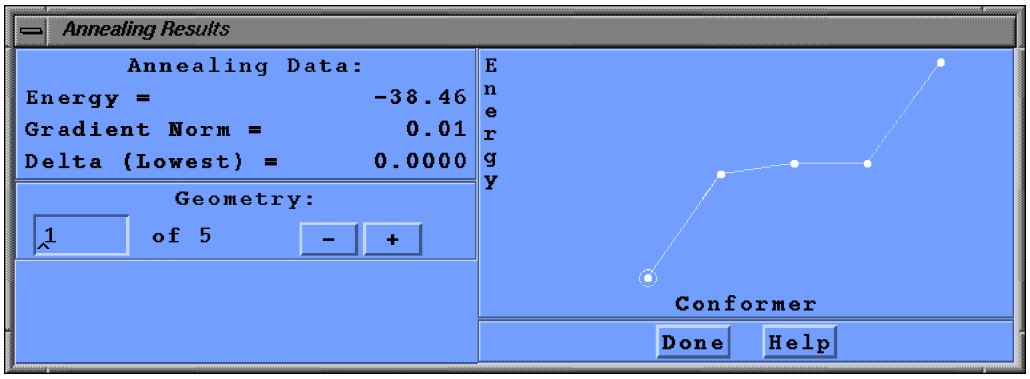
(AMPAC Only) For calculations where a reaction coordinate was performed on one of the geometric parameters, the AMPAC GUI can display the results in graphical format, and this tem on the resuults menu is undimmed. These results may either be from a jobname.OUT, jobname.ARC, or jobname.vis file. For the calculation of the ethane rotational barrier (see TEST09.OUT) the following output is produced:



The energy points (vertical axis) along the "Reaction Coordinate" (horizontal axis) are displayed as located in order from the results file. The "+" and "–" buttons move left and right along the energy display and "Max" moves immediately to the point with the highest computed energy. The "Run" button will automatically cycle through the entire set of points. (The "delay" window is an editable text box that can be used to determine the speed of the cycle. When the cycle reaches either end of the graph, it reverses and follows the reaction coordinate in the other direction.) The information above these buttons corresponds to data from the point being examined (indicated by a circled dot on the display) and the total number of available structures. Particular points may also be selected directly by touching them on the profile plot itself. Note that the displayed geometry changes to reflect the specific point being examined. The "Coordinate" box contains the actual value of the Reaction Coordinate corresponding to the geometry and point selected. "Energy" is the heat of formation (DHf) of this point and "Gradient Norm" is the gradient norm of the geometry. The "Delta (Right)" and "Delta (Left)" values display the difference in energy (kcal/mol) between the present point and those immediately on each side. The "Rxn Gradient" should pass through zero at the maximum on the profile (ostensibly a transition state) and change sign on the other side.

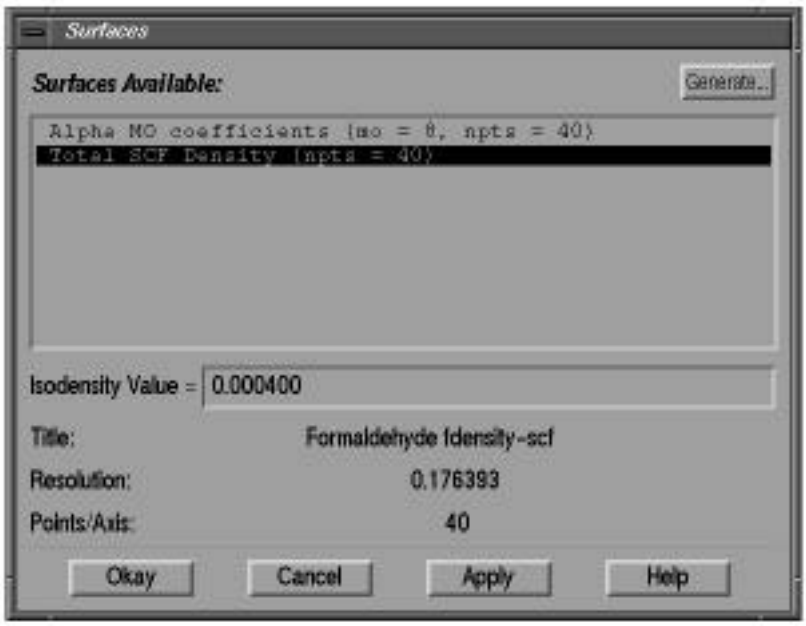
"Annealing....."

(AMPAC Only) For calculations where an annealing search was performed this ietm is undimmed and the AMPAC GUI can display the results in a graphical format similar to the reaction profile. The function of the options on this form are very similar to those as well. These results may either be from a jobname.OUT, jobname.ARC, or jobname.VIS file. A search for the conformers of cyclohexane (see TEST22.OUT) produces the following output:



"Surfaces": Displaying Isosurfaces

The SURFACES option ties the ***AMPAC GUI***'s display capabilities with AMPAC and/or GAUSSIAN-94's ability to write cube files. When a cube file is generated, various chemical data are sampled in three dimensions and written in a specific file formation that the ***AMPAC GUI*** can interpret and display.



Surfaces Dialog Box

"Surfaces Available" Section

This section of the dialog box shows surfaces that are currently available for display. These surfaces are available either after a cube file is opened, or after surfaces are produced using the GENERATE option applied to a checkpoint (.CHK), formatted checkpoint (.FCHK) (GAUSSIAN-94) or an output (.OUT) (AMPAC) file (see below).

"Isodensity Value" Section

Shows the value at which the chemical property of interest will be displayed. This can be varied by the user to change the appearance of the display. (Note that a smaller tolerance value encompasses more volume. The default values for each different type of surface should be correct in most cases.)

"Title" Section

Displays the job's title section as read from the file.

"Resolution" Section

Shows the distance between points in the cube. The value listed here is computed from the number of points requested for the cube divided by the molecular length. Generally, the smaller this distance, the smoother the surface will appear. Also, be aware that the file can grow exponentially in size with increased resolution.

"Points/Axis" Section

Show the number of points per side of the cube file.

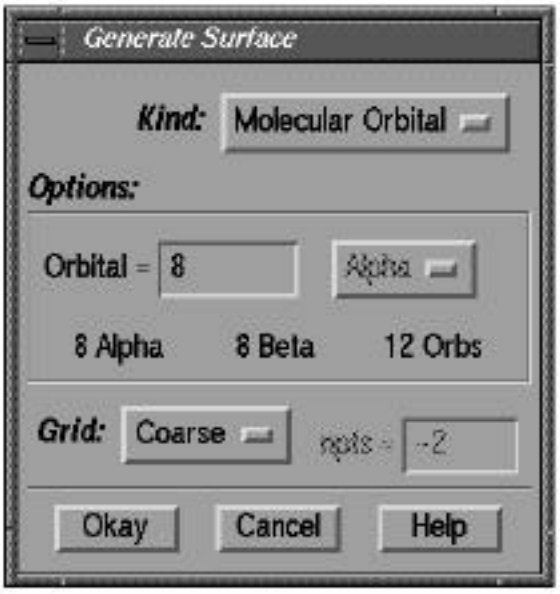
Dialog Box Buttons

The [SURFACES] dialog box buttons are described below.

OK	Builds the selected surface and closes the window.
CANCEL	Stops the procedure and closes the window.
APPLY	Builds the selected surface and leaves the window open.
HELP	Provides on-line information about surfaces.

Generate

The GENERATE option can be used to build new surfaces only if a GAUSSIAN-94 checkpoint or formatted checkpoint file or an AMPAC .OUT file is opened.



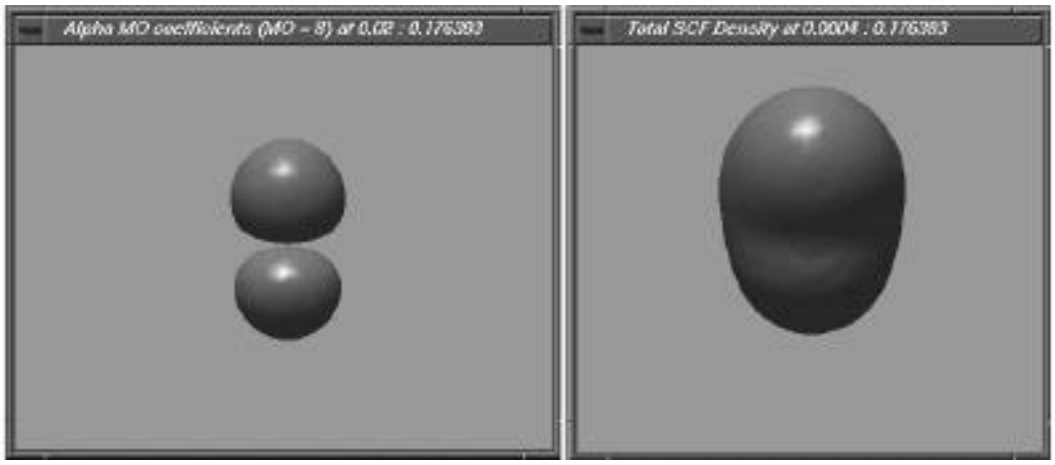
The types of surfaces that you can construct from the data in the file are undimmed on the pop-down menu. Also, various information and additional options are available in the middle section of the dialog box, depending on the type of surface selected.

The quality of the surface can be set using the GRID option as "Coarse", "Medium", "Fine", or "Custom". As the quality of the surface rendered goes up, so does the computational effort required to construct and display it and the disk space and memory to store it. A "Medium" surface should be sufficient for most purposes.

For "Custom" surfaces, you must specify the number of points in the npts text box.

Once all options have been set and the OK button is selected, a background process begins for the construction of the surface. When this surface is available, it will appear on the scrolling list in the [SURFACES] dialog box. *Note: surfaces generated "on the fly" in this manner are not saved to disk and will be lost when the* ***AMPAC GUI*** *terminates.*

Following are some example molecular orbital surfaces:



Molecular Orbital Surface (l) and Electron Density Surface (r)

"View File" Option

This option presents an editor session for the file currently open.

INDEX

—J—

—L—

—M—

—N—

—O—

—P—

—R—

—S—

—T—

—U—

—V—

—W—

—X—

—Z—

—[—